```
=> d his full

     (FILE 'HOME' ENTERED AT 07:42:00 ON 07 JUL 2005)

     FILE 'REGISTRY' ENTERED AT 07:42:09 ON 07 JUL 2005
L1             SCR 1839 AND 1994 AND 2005 AND 1440
L2             SCR 1264
L3             SCR 1210 AND 1263
L4             SCR 1029 OR 1107 OR 1141 OR 1156
L5             STR
L6           18 SEA SSS SAM L5 AND L1 AND (L2 OR L3) AND L4
L7          329 SEA SSS FUL L5 AND L1 AND (L2 OR L3) AND L4
               SAV TEM WARD489F0/A L7
L8             STR L5
L9             STR L8
L10           1 SEA SUB=L7 SSS SAM L9
L11          12 SEA SUB=L7 SSS FUL L9
               SAV TEM L11 WARD489S0/A
L12            STR L9
L13           0 SEA SUB=L7 SSS SAM L12
L14           3 SEA SUB=L7 SSS FUL L12
L15            STR L12
L16           2 SEA SUB=L7 SSS SAM L15
L17          42 SEA SUB=L7 SSS FUL L15
               SAV TEM L17 WARD489S2/A

     FILE 'HCAPLUS' ENTERED AT 08:26:42 ON 07 JUL 2005
               E ROARK WILL/AU
L18          27 SEA ABB=ON  PLU=ON  "ROARK WILLIAM HOWARD"/AU
               E ROARK B/AU
L19        5677 SEA ABB=ON  PLU=ON  (WARNERLAMBERT OR WARNER (1A)LAMBERT?)/CS,P
               A
L20          16 SEA ABB=ON  PLU=ON  L11 OR L14 OR L17
L21           0 SEA ABB=ON  PLU=ON  L20 AND (L18 OR L19)
L22           1 SEA ABB=ON  PLU=ON  US20040224951/PN OR US2002-403037#/AP,PRN

     FILE 'REGISTRY' ENTERED AT 08:29:17 ON 07 JUL 2005

     FILE 'HCAPLUS' ENTERED AT 08:29:19 ON 07 JUL 2005
L23            TRA L22 1- RN :       20 TERMS

     FILE 'REGISTRY' ENTERED AT 08:29:19 ON 07 JUL 2005
L24          20 SEA ABB=ON  PLU=ON  L23
L25          18 SEA ABB=ON  PLU=ON  L24 AND NR>=2
L26          10 SEA ABB=ON  PLU=ON  (NCNC3-NC5 OR NCNC3-NC2NC2 OR NC2SC2-NCNC3
               OR NC2OC2-NCNC3)/ES AND L25
L27           1 SEA ABB=ON  PLU=ON  L26 AND C24H23F2N5O5
L28           4 SEA ABB=ON  PLU=ON  C24H23F2N5O5

     FILE 'HCAPLUS' ENTERED AT 08:38:15 ON 07 JUL 2005
L29           1 SEA ABB=ON  PLU=ON  L26
L30           1 SEA ABB=ON  PLU=ON  L27
L31           1 SEA ABB=ON  PLU=ON  (L29 OR L30) AND (L18 OR L19)
L32             QUE ABB=ON  PLU=ON  PY<=2002 OR PRY<=2002 OR AY<=2002 OR
               PD<20020813 OR PRD<20020813 OR AD<20020813
L33          14 SEA ABB=ON  PLU=ON  L32 AND L20
L34          16 SEA ABB=ON  PLU=ON  L20 OR L33

     FILE 'HCAOLD' ENTERED AT 08:41:31 ON 07 JUL 2005
L35           5 SEA ABB=ON  PLU=ON  L11 OR L14 OR L17
               SEL AN
               EDIT E1-E5 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 08:42:02 ON 07 JUL 2005
L36           7 SEA ABB=ON  PLU=ON  ("CA57:8574C"/OREF OR "CA59:6420H"/OREF OR
               "CA61:7024H"/OREF OR "CA61:7025B"/OREF OR "CA63:7781H"/OREF)
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L37           7 SEA ABB=ON  PLU=ON  L36 AND L32
L38          21 SEA ABB=ON  PLU=ON  L34 OR L37

     FILE 'HCAOLD' ENTERED AT 08:43:09 ON 07 JUL 2005
               SEL HIT RN L35

     FILE 'REGISTRY' ENTERED AT 08:43:18 ON 07 JUL 2005
L39           7 SEA ABB=ON  PLU=ON  (96732-27-3/RN OR 3215-22-3/RN OR 3215-23-4
                /RN OR 93738-69-3/RN OR 95709-04-9/RN OR 96732-25-1/RN OR
                97864-53-4/RN)

     FILE 'HCAOLD' ENTERED AT 08:43:44 ON 07 JUL 2005
L40           0 SEA ABB=ON  PLU=ON  (L26 OR L27)

=> b reg

FILE 'REGISTRY' ENTERED AT 08:44:07 ON 07 JUL 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     6 JUL 2005  HIGHEST RN 853990-77-9
DICTIONARY FILE UPDATES:    6 JUL 2005  HIGHEST RN 853990-77-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d que sta l11
L1            SCR 1839 AND 1994 AND 2005 AND 1440
L2            SCR 1264
L3            SCR 1210 AND 1263
L4            SCR 1029 OR 1107 OR 1141 OR 1156
L5            STR
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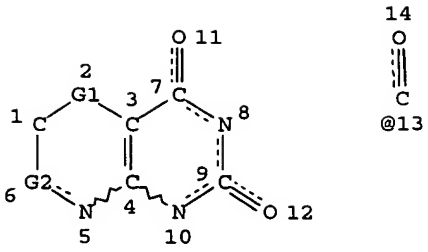
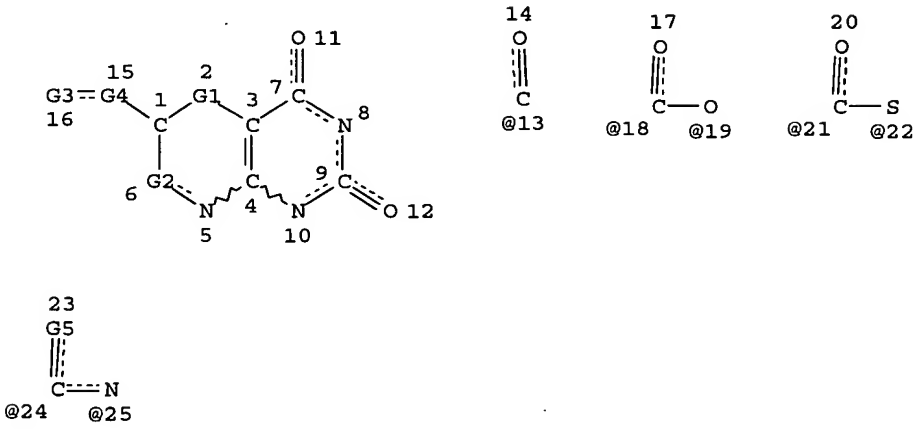


VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L7 329 SEA FILE=REGISTRY SSS FUL L5 AND L1 AND (L2 OR L3) AND L4
L9 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
VAR G3=AK/CY
VAR G4=CY/18-1 19-16/18-16 19-1/21-1 22-16/21-16 22-1/24-1 25-16/25-1 24-16
VAR G5=O/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L11 12 SEA FILE=REGISTRY SUB=L7 SSS FUL L9

100.0% PROCESSED 329 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

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=> d que sta l14
L1              SCR 1839 AND 1994 AND 2005 AND 1440
L2              SCR 1264
L3              SCR 1210 AND 1263
L4              SCR 1029 OR 1107 OR 1141 OR 1156
L5              STR
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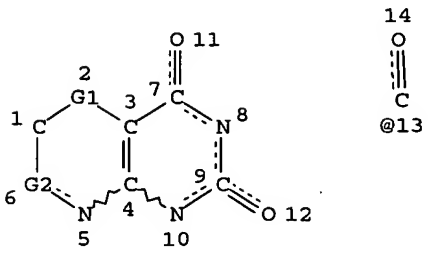


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VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L7          329 SEA FILE=REGISTRY SSS FUL L5 AND L1 AND (L2 OR L3) AND L4
L12             STR
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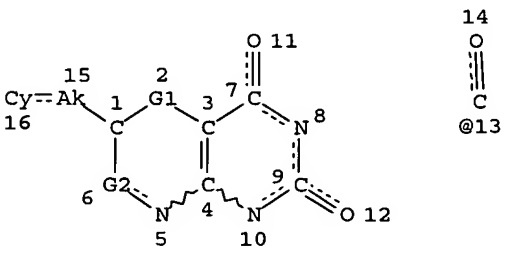


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VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE
L14           3 SEA FILE=REGISTRY SUB=L7 SSS FUL L12

100.0% PROCESSED     329 ITERATIONS                          3 ANSWERS
SEARCH TIME: 00.00.01


=> d que sta l17
L1              SCR 1839 AND 1994 AND 2005 AND 1440
L2              SCR 1264
L3              SCR 1210 AND 1263
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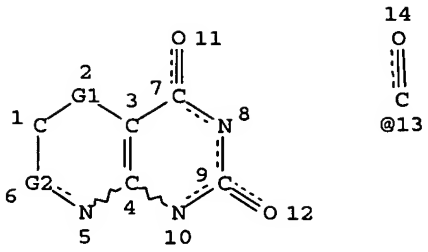
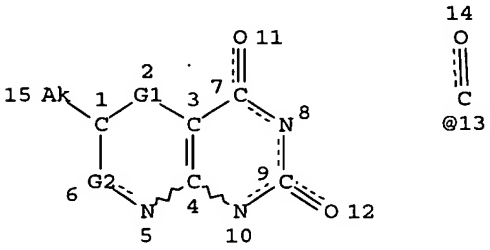
L4 SCR 1029 OR 1107 OR 1141 OR 1156
L5 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L7 329 SEA FILE=REGISTRY SSS FUL L5 AND L1 AND (L2 OR L3) AND L4
L15 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

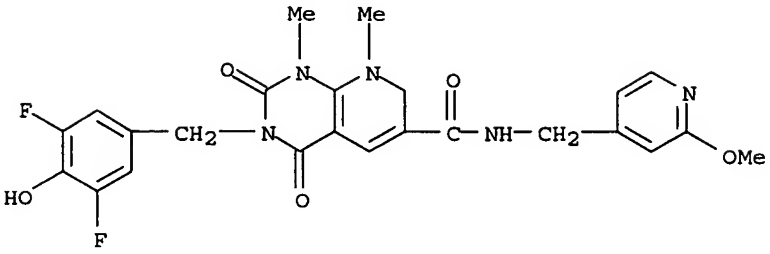
STEREO ATTRIBUTES: NONE
L17 42 SEA FILE=REGISTRY SUB=L7 SSS FUL L15

100.0% PROCESSED 329 ITERATIONS 42 ANSWERS
SEARCH TIME: 00.00.01

=> d ide l27

L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN **657351-04-7** REGISTRY
ED Entered STN: 03 Mar 2004
CN Pyrido[2,3-d]pyrimidine-6-carboxamide, 3-[(3,5-difluoro-4-hydroxyphenyl)methyl]-1,2,3,4,7,8-hexahydro-N-[(2-methoxy-4-pyridinyl)methyl]-1,8-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C24 H23 F2 N5 O5
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> b hcap
FILE 'HCAPLUS' ENTERED AT 08:44:35 ON 07 JUL 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 7 Jul 2005 VOL 143 ISS 2
FILE LAST UPDATED: 6 Jul 2005 (20050706/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all fhitstr l31 tot

L31 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:143163 HCAPLUS
DN 140:175195
ED Entered STN: 22 Feb 2004
TI 5,6-Fused uracil derivatives as matrix metalloproteinase inhibitors, pharmaceutical compositions, and therapeutic use
IN **Roark, William Howard**
PA **Warner-Lambert** Company LLC, USA
SO PCT Int. Appl., 193 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D495-04
ICS C07D471-04; A61K031-519; A61P019-02
CC 1-12 (Pharmacology)

Section cross-reference(s): 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004014921	A1	20040219	WO 2003-IB3505	20030804
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004224951	A1	20041111	US 2003-634489	20030805
PRAI	US 2002-403037P	P	20020813		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004014921	ICM	C07D495-04
	ICS	C07D471-04; A61K031-519; A61P019-02
WO 2004014921	ECLA	C07D471/04+239B+221B; C07D495/04+335B+239B
US 2004224951	NCL	514/242.000; 514/262.100; 514/264.100; 544/184.000; 544/256.000; 544/279.000
	ECLA	C07D471/04+239B+221B; C07D495/04+335B+239B

OS MARPAT 140:175195

AB The invention provides 5,6-fused uracil derivs.,or pharmaceutically acceptable salts thereof. The invention also provides pharmaceutical compns. comprising a compound of the invention, or a pharmaceutically acceptable salt thereof, together with a pharmaceutically acceptable carrier, diluent, or excipient. The invention also provides methods of inhibiting a MMP-13 enzyme in an animal, comprising administering a compound of the invention, or a pharmaceutically acceptable salt thereof. The invention also provides methods of treating a disease mediated by an MMP-13 enzyme in a patient, comprising administering to the patient a compound of the invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition The invention also provides methods of treating diseases such as heart disease, multiple sclerosis, osteo- and rheumatoid arthritis, arthritis other than osteo- or rheumatoid arthritis, cardiac insufficiency, inflammatory bowel disease, heart failure, age-related macular degeneration, chronic obstructive pulmonary disease, asthma, periodontal diseases, psoriasis, atherosclerosis, and osteoporosis in a patient, comprising administering to the patient a compound of the invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition The invention also provides combinations, comprising a compound of the invention, or a pharmaceutically acceptable salt thereof, together with another pharmaceutically active component.

ST fused uracil deriv matrix metalloproteinase inhibitor therapeutic

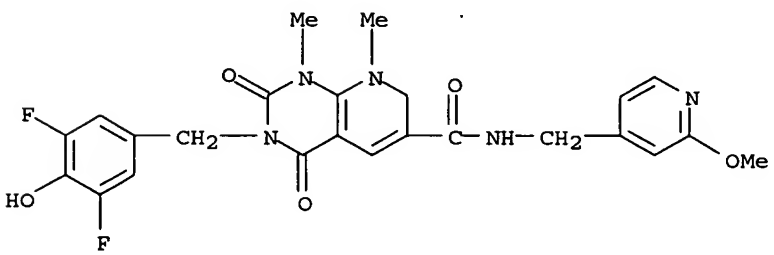
IT Drug delivery systems
(capsules; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Ampuls
Antiarthritics
Arthritis
Drug delivery systems
Human
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(injections; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(ointments; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

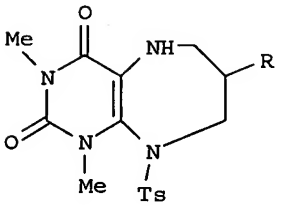
IT Drug delivery systems
(solns.; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT Drug delivery systems
(suppositories; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT Drug delivery systems
(tablets, coated; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT Drug delivery systems
(tablets; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT 141907-41-7, Matrix metalloproteinase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT 657350-98-6 657350-99-7 657351-00-3 657351-01-4 657351-02-5
657351-03-6 **657351-04-7** **657351-05-8**
657351-06-9 **657351-07-0** **657351-08-1**
657351-09-2 **657351-10-5** **657351-11-6**
657351-12-7 **657351-13-8**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
IT 169590-42-5, Celecoxib 181695-72-7, Valdecoxib
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., therapeutic use, and use with other agents)
IT 329900-75-6, Cyclooxygenase 2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., therapeutic use, and use with other agents)
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Ibfb Gmbh; DE 10101324 C 2001 HCAPLUS
(2) Ibfb Gmbh; DE 19940494 C 2001 HCAPLUS
(3) Warner-Lambert Company; WO 02064572 A 2002 HCAPLUS
(4) Warner-Lambert Company; WO 02064598 A 2002 HCAPLUS
(5) Warner-Lambert Company; WO 03033477 A 2003 HCAPLUS
(6) Warner-Lambert Company; WO 03033478 A 2003 HCAPLUS
IT **657351-04-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)
RN 657351-04-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxamide, 3-[(3,5-difluoro-4-hydroxyphenyl)methyl]-1,2,3,4,7,8-hexahydro-N-[(2-methoxy-4-pyridinyl)methyl]-1,8-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



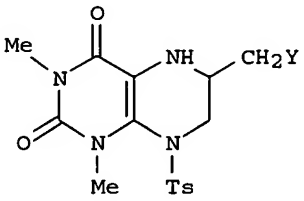
Search done by Noble Jarrell

=> d all hitstr l38 tot

L38 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:865843 HCAPLUS
DN 140:59606
ED Entered STN: 05 Nov 2003
TI Synthesis of the tetrahydropteridine-2,4-dione having a substituted methyl group at 6-position
AU Tada, Masaru; Shimamura, Tomoyuki; Suzuki, Takeaki
CS Department of Chemistry, School of Science and Engineering, Waseda University, Tokyo, 169-8555, Japan
SO Heterocycles (2003), 60(11), 2511-2517
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 140:59606
GI



I



II

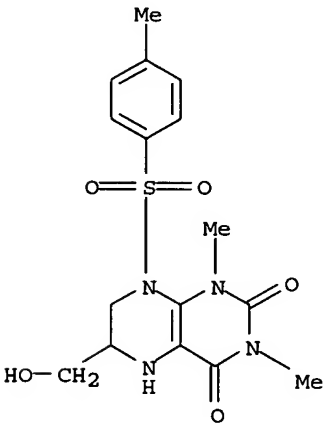
AB Lewis acid treatment of 5-amino-6-(N-2,3-epoxypropyl-N-tosyl)amino-1,3-dimethyluracil gave the diazepine (I, R = OH), and the tosylate (I, R = OTs) from this compound underwent ring transformation to provide tetrahydropteridinediones (II, Y = OTs, OH) depending on the reaction conditions. Thus, heating in dry acetonitrile led to 6-tosyloxymethyl-tetrahydropteridine-2,4-dione (II, Y = OTs), whereas in wet acetonitrile, the 6-hydroxymethyl derivative (II, Y = OH) was obtained.
ST tetrahydropteridinedione prepn
IT 1203-25-4 5997-56-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetrahydropteridine-2,4-dione having a substituted Me group at 6-position)
IT 638212-21-2P 638212-22-3P 638212-23-4P 638212-24-5P
638212-26-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrahydropteridine-2,4-dione having a substituted Me group at 6-position)
IT **638212-25-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrahydropteridine-2,4-dione having a substituted Me group at 6-position)
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Al-Sehemi, A; J Chem Soc, Perkin Trans 1 2000, P4413 HCAPLUS
(2) Bailey, S; J Org Chem 1992, V57, P4470 HCAPLUS
(3) Boyle, P; J Chem Res, Synop 1989, P282 HCAPLUS
(4) Boyle, P; Miniprint 1989, P2086
(5) Brown, D; ` Fused Pyrimidines,' Part 3 1988, P267 MEDLINE
(6) Brown, D; ` Fused Pyrimidines,' Part 3 1988, P43
(7) Clayden, J; J Chem Soc Perkin Trans 1 2000, P3232 HCAPLUS

(8) Curran, D; J Am Chem Soc 1994, V116, P3131 HCAPLUS
(9) Dimarco, A; Ann Rev Biochem 1990, V59, P355 HCAPLUS
(10) Liao, T; J Heterocycl Chem 1964, V1, P212 HCAPLUS
(11) Matsuura, S; Bull Chem Soc Jpn 1981, V54, P2543 HCAPLUS
(12) Pfleiderer, W; Comprehensive Heterocyclic Chemistry 1984, V3(Part 2B), P325
(13) Temple, C; Chemistry and Biochemistry of Folates 1984, V1, P61 HCAPLUS
(14) Tulinsky, J; J Org Chem 1999, V64, P93 HCAPLUS

IT **638212-26-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrahydropteridine-2,4-dione having a substituted Me group at 6-position)

RN 638212-26-7 HCAPLUS

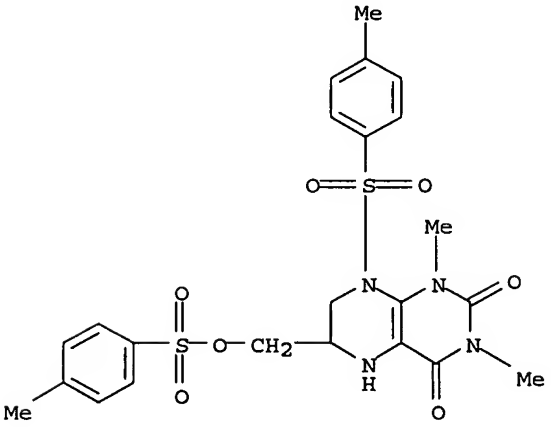
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-6-(hydroxymethyl)-1,3-dimethyl-8-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



IT **638212-25-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrahydropteridine-2,4-dione having a substituted Me group at 6-position)

RN 638212-25-6 HCAPLUS

CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3-dimethyl-8-[(4-methylphenyl)sulfonyl]-6-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (9CI) (CA INDEX NAME)



Search done by Noble Jarrell

L38 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:721630 HCAPLUS
DN 140:16703
ED Entered STN: 15 Sep 2003
TI Cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines
AU Kolos, Nadezhda; Beryozkina, Tatyana; Orlov, Valeriy
CS Department of Organic Chemistry, V. N. Karazin Kharkiv National University, Kharkov, 61077, Ukraine
SO Heterocycles (2003), 60(9), 2115-2122
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 140:16703
AB Reaction of β-aroylacrylic acids with 2,3-diaminopyridine, 5,6-diamino-1,3-dimethyluracil, and 2,5,6-triamino-4-oxopyrimidine was studied. 1,3-Dimethyl-5,8-dihydro-1H,3H,6H-pteridine-2,4,7-trione and 2-amino-4-hydroxy-6-(2-oxo-2-phenylethyl)-5,8-dihydro-6H-pteridin-7-one were rearranged into pteridin-6-ylideneacetic acids. Reaction of α,β-dibromo-β-benzoylpropionic acid with 5,6-diamino-1,3-dimethyluracil led to 8-benzoylpurine via the formation of an enamino ketone.0.
ST cyclocondensations aroylacrylic acid heterocyclic diamine
IT Cyclocondensation reaction
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(diamines; cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
IT 452-58-4, 2,3-Diaminopyridine 583-06-2 5440-00-6, 5,6-Diamino-1,3-dimethyluracil 6269-33-6 24849-45-4 51324-37-9 99074-11-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
IT **629627-80-1P** 629627-81-2P 629627-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
IT **629627-78-7P 629627-79-8P** 629627-82-3P 629627-83-4P 629627-84-5P 629627-85-6P 629627-86-7P 629627-87-8P 629627-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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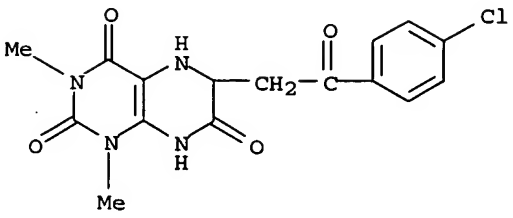
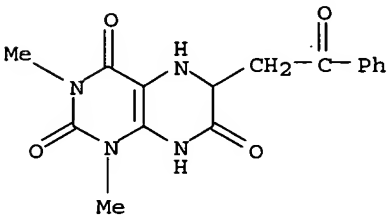
IT **629627-80-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
RN 629627-80-1 HCAPLUS
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 6-[2-(4-chlorophenyl)-2-oxoethyl]-5,8-

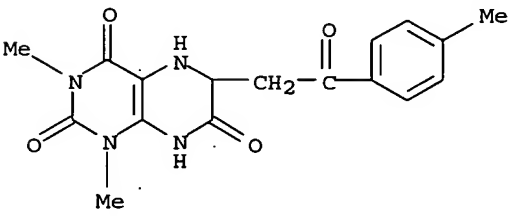
dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



IT **629627-78-7P 629627-79-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclocondensations of β-aroylacrylic acids with heterocyclic O-diamines)
RN 629627-78-7 HCAPLUS
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3-dimethyl-6-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)



RN 629627-79-8 HCAPLUS
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3-dimethyl-6-[2-(4-methylphenyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)



L38 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:466940 HCAPLUS
DN 136:134727
ED Entered STN: 28 Jun 2001
TI Behavior of enaminouracil Mannich base towards nucleophiles
AU Hamama, W. S.; Zoorob, H. H.
CS Chemistry Department, Faculty of Science, Mansoura University, Mansoura, Egypt
SO Mansoura Science Bulletin, A: Chemistry (2001), 28(Suppl. 1), 99-110
CODEN: MSBCF4; ISSN: 1110-4562
PB Mansoura University
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 136:134727
AB C-Alkylations of enaminouracil Mannich base with heterocyclic nucleophiles

such as indole, antipyrine, 1,3-dimethyl-6-aminouracil, creatinine, 1,3-dimethylbarbituric acid or saccharin to synthesize the corresponding heterocycles were accomplished. Transamination of the starting compound with ammonium carbonate was successful. Furthermore, the behavior of the starting compound towards aliphatic nucleophiles such as malononitrile, cyanoacetamide, cyanoacetohydrazide, 2-cyanomethylenebenzimidazole, malonic ester, and Ph acetic ester gave pyrido[2,3-d]pyrimidine derivative

ST alkylation cyclization enaminouracil Mannich base nucleophile; pyridopyrimidine prepn

IT Alkylation
Cyclization
Nucleophiles
(C-alkylation and cyclization of enaminouracil Mannich base with nucleophiles)

IT 60-27-5, Creatinine 60-80-0, Antipyrine 81-07-2, Saccharin 101-97-3, Ethyl phenylacetate 105-53-3, Diethyl malonate 107-91-5, Cyanoacetamide 109-77-3, Malononitrile 120-72-9, Indole, reactions 140-87-4, Cyanoacetohydrazide 769-42-6, 1,3-Dimethylbarbituric acid 4414-88-4, 1H-Benzimidazole-2-acetonitrile 6642-31-5, 1,3-Dimethyl-6-aminouracil 286434-39-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(C-alkylation and cyclization of enaminouracil Mannich base with nucleophiles)

IT 10146-98-2P 393108-20-8P 393108-21-9P 393108-22-0P 393108-23-1P 393108-24-2P 393108-25-3P 393108-26-4P 393108-27-5P 393108-28-6P 393108-29-7P **393108-30-0P** 393108-31-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(C-alkylation and cyclization of enaminouracil Mannich base with nucleophiles)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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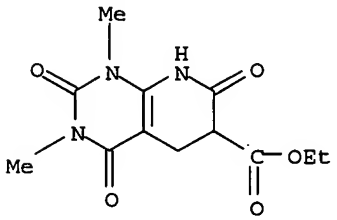
IT **393108-30-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(C-alkylation and cyclization of enaminouracil Mannich base with nucleophiles)

RN 393108-30-0 HCAPLUS

CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,7-trioxo-, ethyl ester (9CI) (CA INDEX NAME)



L38 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:83454 HCAPLUS

DN 132:302955

ED Entered STN: 04 Feb 2000

TI Antitumoral activity of new pyrimidine derivatives of sesquiterpene lactones

AU Quintero, Angelina; Pelcastre, Araceli; Solano, Jose Dolores; Guzman, Angel; Diaz, Eduardo

CS Facultad de Quimica, Universidad Nacional autonoma de Mexico, Ciudad Universitaria, Coyoacan, 04510, Mex.

SO Journal of Pharmacy & Pharmaceutical Sciences [Electronic Publication] (1999), 2(3), 108-122
CODEN: JPPSFY; ISSN: 1482-1826
URL: http://www.ualberta.ca/~csps/JPPS2(3)/A.Quintero/antitumoral.htm

PB Canadian Society for Pharmaceutical Sciences

DT Journal; (online computer file)

LA English

CC 1-3 (Pharmacology)

AB Sesquiterpene lactones display a wide variety of biol. effects such as antiviral, anti-inflammatory and cytotoxic activity. In previous studies some derivs. of sesquiterpene lactones were prepared to be tested as antiviral and/or cytotoxic agents. In the present report we describe the effects of seven modified sesquiterpene lactones on the proliferation of several cancer cell lines. We demonstrated antitumor activity of two of them: III (JLNZ-106) and IV (EDAG-IV-Sme) in HeLa, C-33, CALO, INBL, VIPA, SW480, SW620, MCF-7 and CHO cancer cell lines. Compds. III (JLNZ-106) and IV (EDAG-IV-Sme-IV) presented cytotoxic activity (IC50) by inhibiting the incorporation of 14C-thymidine to DNA. These expts. suggest that derivs. III and IV should inhibit DNA replication in cancer cell lines.

ST pyrimidine deriv sesquiterpene lactone antitumor SAR

IT Natural products, pharmaceutical
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of new pyrimidine derivs. of sesquiterpene lactones)

IT Structure-activity relationship
(antitumor; antitumor activity of new pyrimidine derivs. of sesquiterpene lactones)

IT Sesquiterpenes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lactones; antitumor activity of new pyrimidine derivs. of sesquiterpene lactones)
IT 192509-97-0 **192509-98-1** 204066-92-2 207113-29-9
207113-30-2 207113-32-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of new pyrimidine derivs. of sesquiterpene lactones)
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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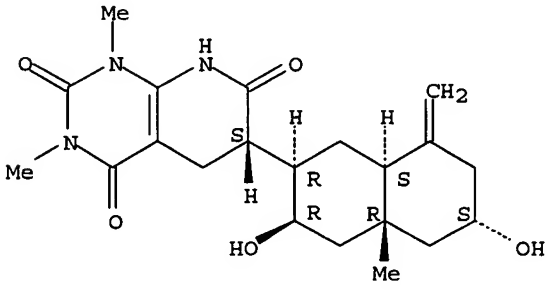
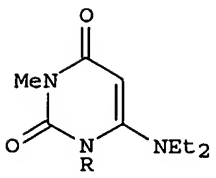
(12) Woerdenbang, H; Planta Medica 1994, V60, P434
IT **192509-98-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of new pyrimidine derivs. of sesquiterpene lactones)
RN 192509-98-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[(2R,3R,4aR,6S,8aS)-decahydro-3,6-dihydroxy-4a-methyl-8-methylene-2-naphthalenyl]-5,8-dihydro-1,3-dimethyl-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L38 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:598911 HCAPLUS
DN 130:81474
ED Entered STN: 22 Sep 1998
TI Studies on Uracils: Synthesis of Novel Uracil Analogs via 1,5- and 1,6-Intramolecular Cycloaddition Reactions
AU Bhuyan, Pulak J.; Lekhok, Kushal C.; Sandhu, Jagir S.
CS Regional Research Laboratory, Jorhat, 785-006, India
SO Journal of Chemical Research, Synopses (1998), (9), 502-503, 2025-2032
CODEN: JRPSDC; ISSN: 0308-2342
PB Royal Society of Chemistry

DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
GI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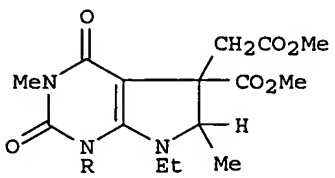
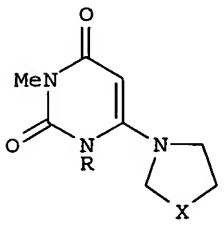
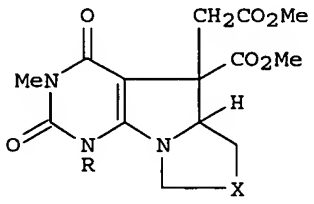

II


III


IV

AB 6-(Tertiary amino)uracils I (R = Me, H) react with di-Me acetylenedicarboxylate to afford 5,6-dihydropyrrolo[2,3-d]pyrimidines II, and uracils III (R = Me, H; X = CH2, CH2CH2) react with di-Me acetylenedicarboxylate to afford tricyclic compds. IV via 1,5-electrocyclization in excellent yields. suitably functionalized uracil derivs. 5. Uracils functionalized with a 2,2-dicyanovinyl group undergo intramol. 1,6-cycloaddn. reactions to afford 5,6,7,8-tetrahydropyrido[2,3-d]pyrimidines and tricyclic analogs in high yields.

ST uracil electrocyclization acetylenedicarboxylate; cycloaddn intramol uracil dicyanovinyl deriv; pyrrolopyrimidine deriv prepn; pyridopyrimidine deriv prepn

IT Cyclization
(electrocyclic, 1,5-; uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

IT Cycloaddition reaction
(intramol., 1,6-; uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

IT 109-77-3, Malononitrile 109-89-7, reactions 123-75-1, Pyrrolidine, reactions 762-42-5, Dimethyl acetylenedicarboxylate 6972-27-6, 6-Chloro-1,3-dimethyluracil 35824-85-2 176214-30-5 218447-53-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

IT 74151-85-2P 74151-86-3P 155544-40-4P 193696-10-5P 193696-12-7P 193696-16-1P 193696-18-3P 193696-20-7P 218447-54-2P 218447-55-3P 218447-57-5P 218447-58-6P 218447-59-7P 218447-60-0P 218447-61-1P 218447-62-2P 218447-63-3P 218447-64-4P 218447-65-5P 218447-66-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

IT 176214-27-0P 176214-29-2P 184290-20-8P 184290-21-9P 193696-29-6P 193696-31-0P 218447-67-7P 218447-70-2P 218447-72-4P 218447-73-5P **218447-74-6P** **218447-75-7P** 218447-76-8P 218447-77-9P 218447-78-0P 218447-79-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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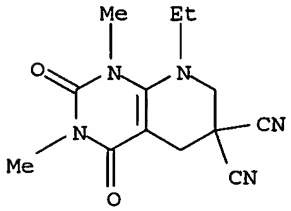
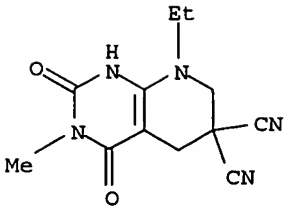
IT **218447-74-6P 218447-75-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(uracil analogs via 1,5-electrocyclization and 1,6-intramol. cycloaddn. reactions)

RN 218447-74-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6,6(2H)-dicarbonitrile, 8-ethyl-1,3,4,5,7,8-hexahydro-1,3-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 218447-75-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6,6(2H)-dicarbonitrile, 8-ethyl-1,3,4,5,7,8-hexahydro-3-methyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L38 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:231734 HCAPLUS
DN 128:321761
ED Entered STN: 25 Apr 1998
TI 2D 1H and 13C NMR evidence for stereoselective formation of a new bond C-N, C-S or C-C in reaction of ivalin acetate with substituted pyrimidines
AU Diaz, E.; Nava, J. L.; Barrios, H.; Quiroz, B.; Guzman, A.; Leon G., L.; Fuentes B., A.
CS Instituto de Quimica, Circuito Exterior Ciudad Univer., University Nacional Autonoma de Mexico, 04410, Mex.
SO Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1998), 54A(4), 567-574
CODEN: SAMCAS; ISSN: 0584-8539
PB Elsevier Science B.V.
DT Journal
LA English
CC 30-15 (Terpenes and Terpenoids)
Section cross-reference(s): 22, 26
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Several pyrimidine derivs., e.g. I, II (R = H, R1 = H, Me, Br, F, R2 = Ac, X = Y = O; R = H, R1 = OMe, Me, R2 = Ac, X = S, Y = O; R = R2 = H, R1 = CH2OH, X = Y = O; R = CH2CHMe2, R1 = CF3, R2 = Ac, X = Y = O) and III of ivalin acetate were synthesized as potential anti HIV agents. High stereoselective Michael addition to ivalin acetate was observed and a new C-C, C-N or C-S bond was formed. 2D NMR 1H and 13C as well as X-ray crystallog. studies were performed on the compds. herein described to established the structure and stereochem.
ST ivalin acetate Michael addn pyrimidine base; NMR ivalin pyrimidine adduct structure stereochem
IT Michael reaction
NMR (nuclear magnetic resonance)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)
IT Pyrimidine bases
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)
IT Sesquiterpenes
RL: RCT (Reactant); RACT (Reactant or reagent)
(eudesmanolides; NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)
IT 192509-99-2P 207113-25-5P 207113-26-6P 207113-27-7P
207113-28-8P 207113-29-9P 207113-30-2P 207113-31-3P 207113-32-4P
207113-33-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)
IT 51-20-7, 5-Bromouracil 51-21-8, 5-Fluorouracil 65-71-4, 5-Methyluracil

66-22-8, Uracil, reactions 636-26-0, 5-Methyl-2-thiouracil 4433-40-3, 5-(Hydroxymethyl)uracil 5938-03-4, Ivalin 6642-31-5, 6-Amino-1,3-dimethyl-2,4-pyrimidinedione 6939-11-3, 5-Methoxy-2-thiouracil 199444-79-6, 3-Isobutyl-5-(trifluoromethyl)uracil
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)

IT 60109-20-8P, Ivalin acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(2) Bax, A; J Am Chem Soc 1986, V108, P2093 HCAPLUS
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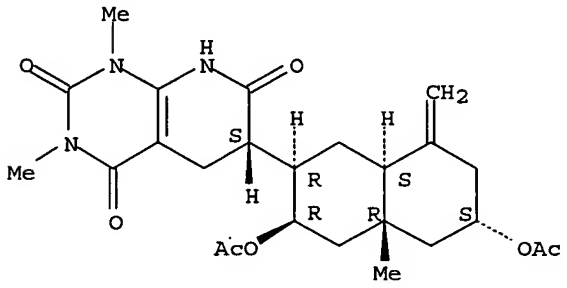
(21) Tarek, S; Med Chem Res 1995, V5, P417

IT **192509-99-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NMR evidence for stereoselective formation in reaction of ivalin acetate with substituted pyrimidines)

RN 192509-99-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[(2R,3R,4aR,6S,8aS)-3,6-bis(acetyloxy)decahydro-4a-methyl-8-methylene-2-naphthalenyl]-5,8-dihydro-1,3-dimethyl-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L38 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:458961 HCAPLUS
DN 127:121888
ED Entered STN: 23 Jul 1997
TI Stereoselective Michael addition of 6-amino-1,3-dimethyl-2,4-pyrimidinedione to the exocyclic methylene of three sesquiterpene

lactones. 1H and 13C NMR evidence of a new C-C bond and lactam formation
AU Diaz, Eduardo; Barrios, Hector; Nava, Jose Luis; Enriquez, Raul G.; Guzman, Angel; Leon G., Leticia; Fuentes, Fernando; Fuentes B., Aidee; Quintero, Angelina; Solano, Jose Dolores
CS Instituto de Quimica, Universidad Nacional Autonoma de Mexico, Circuito Exterior, Ciudad Universitaria, Coyoacan, 04510, Mex.
SO Journal of Heterocyclic Chemistry (1997), 34(3), 1037-1041
CODEN: JHTCAD; ISSN: 0022-152X
PB HeteroCorporation
DT Journal
LA English
CC 30-15 (Terpenes and Terpenoids)
OS CASREACT 127:121888
AB The stereoselective addition of 6-amino-1,3-dimethyl-2,4-pyrimidinedione to the exocyclic methylene of the α,β unsatd. dehydrocostus lactone, Ivalin acetate (I) and Zaluzanin A diacetate (II), was achieved resulting in a new C-C bond formation. In the cases of compds. I and II, after the addition, the lactone was cleaved followed by reclosure into a lactam ring system.
ST stereoselective Michael addn sesquiterpene pyrimidinedione aminodimethyl; dehydrocostus lactone aminodimethylpyrimidinedione stereoselective Michael addn; Ivalin acetate aminodimethylpyrimidinedione stereoselective Michael addn; Zaluzanin A diacetate stereoselective Michael addn
IT Sesquiterpenes
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
IT Michael reaction
(stereoselective; stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
IT 477-43-0, Dehydrocostus lactone 6642-31-5 14026-81-4, Zaluzanin A acetate 60109-20-8, Ivalin acetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
IT **192509-98-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
IT **192509-97-0P 192509-99-2P 192510-00-2P 192510-01-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Alley, M; Cancer Res 1988, V48, P589 MEDLINE
(2) Balzarini, J; Design of Anti-Aids Drugs 1990, P175 HCAPLUS
(3) Carmichael, J; Cancer Res 1987, V47, P936 HCAPLUS
(4) Chapman; Dictionary of Organic Compounds
(5) de Clercq, E; Antiviral Res 1987, V8, P261 HCAPLUS
(6) de Lange, B; Tetrahedron 1989, V45, P6799 HCAPLUS
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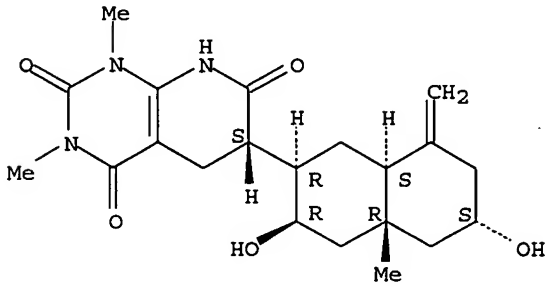
(10) Hayashi, S; Antimicrob Agents Chemother 1990, V34, P287 HCAPLUS
(11) Hoshino, H; J Antibiotics 1987, V40, P1077 HCAPLUS
(12) Krafft, M; Tetrahedron Letters 1986, V27, P2087 HCAPLUS
(13) Li, Y; Phytochemistry 1989, V28, P3395 HCAPLUS
(14) Marco, J; Tetrahedron Letters 1991, V32, P5193 HCAPLUS
(15) Mulzer, J; Tetrahedron Asymmetry 1993, V4, P457 HCAPLUS
(16) Norbeck, O; J Med Chem 1990, V33, P1285
(17) Park, B; J Antibiot 1988, V41, P751 HCAPLUS
(18) Parlmutter, P; Organic Synthesis 1992, P283

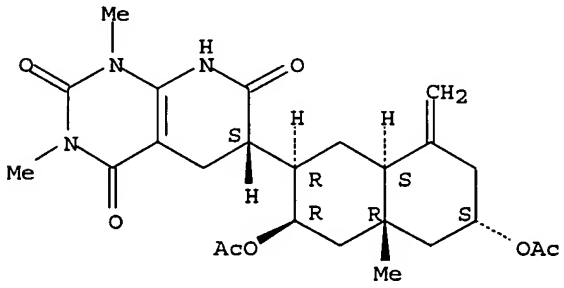
IT 192509-98-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
RN 192509-98-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[(2R,3R,4aR,6S,8aS)-decahydro-3,6-dihydroxy-4a-methyl-8-methylene-2-naphthalenyl]-5,8-dihydro-1,3-dimethyl-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



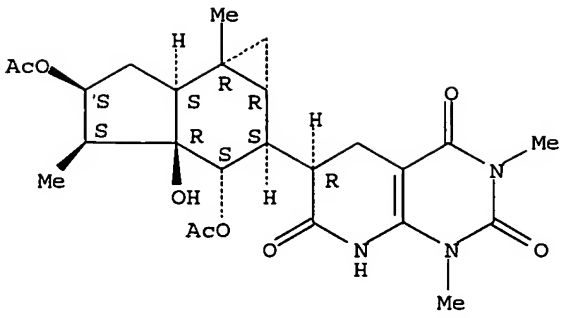
IT 192509-99-2P 192510-00-2P 192510-01-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective Michael addition of aminodimethylpyrimidinedione to the exocyclic methylene of three sesquiterpene lactones)
RN 192509-99-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[(2R,3R,4aR,6S,8aS)-3,6-bis(acetyloxy)decahydro-4a-methyl-8-methylene-2-naphthalenyl]-5,8-dihydro-1,3-dimethyl-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



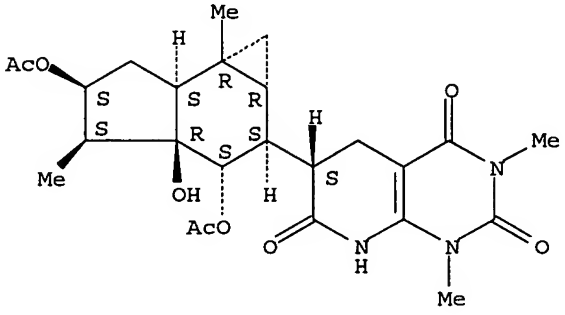
RN 192510-00-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[3,5-bis(acetyloxy)decahydro-3a-hydroxy-4,6b-dimethylcycloprop[e]inden-2-yl]-5,8-dihydro-1,3-dimethyl-, [1aR-[1aα,2α(R*),3β,3aα,4α,5α,6aβ,6bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

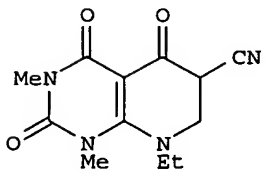


RN 192510-01-3 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 6-[3,5-bis(acetyloxy)decahydro-3a-hydroxy-4,6b-dimethylcycloprop[e]inden-2-yl]-5,8-dihydro-1,3-dimethyl-, [1aR-[1aα,2α(S*),3β,3aα,4α,5α,6aβ,6bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L38 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:796882 HCAPLUS
DN 124:29695
ED Entered STN: 16 Sep 1995
TI Synthesis and biological activity of 8-alkyl(aryl)-6-cyanopyrido[2,3-d]pyrimidine-2,4,5-triones
AU Skudarnova, T. I.; Burova, O. A.; Smirnova, N. M.; Chelysheva, G. M.; Safonova, T. S.
CS Novokuznetsk. Nauchno-Issled. Khim.-Farm. Inst., Novokuznetsk, Russia
SO Khimiko-Farmatsevticheskii Zhurnal (1994), 28(3), 39-42
CODEN: KHFZAN; ISSN: 0023-1134
PB Meditsina
DT Journal
LA Russian
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
GI



I

AB The title compds., e.g., I, were prepared by reaction of 1,3-dimethyl-5-(cyanoacetyl)-6-(substituted amino)uracils with amide acetals. Hydrolysis of the nitriles to the carboxylic acids and amides was studied. The compds. were tested for antibacterial activity.

ST pyridopyrimidinetrione cyano prepn hydrolysis antibacterial activity; hydrolysis cyanopyridopyrimidinetrione; bactericide pyridopyrimidinetrione carboxylic acid amide nitrile

IT Bactericides, Disinfectants, and Antiseptics
(pyridopyrimidinetriones)

IT **171507-46-3P 171507-52-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

IT 171507-48-5P 171507-54-3P **171507-55-4P** 171507-56-5P **171507-57-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

IT 1188-33-6, DMF diethyl acetal 19429-85-7, Acetamide, N,N-dimethyl-, diethyl acetal 132373-28-5 132373-29-6 137278-06-9 171507-43-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

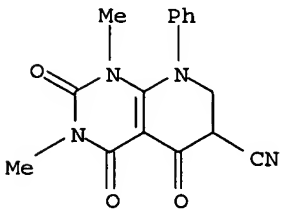
IT **171507-44-1P** 171507-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

IT 37587-44-3P **171507-45-2P 171507-47-4P** 171507-49-6P 171507-51-0P **171507-53-2P** 171507-58-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

IT **171507-46-3P 171507-52-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)

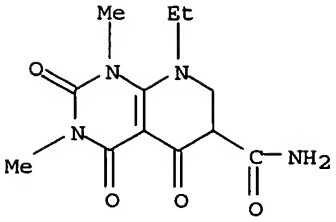
RN 171507-46-3 HCAPLUS

CN Pyrido[2,3-d]pyrimidine-6-carbonitrile, 1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo-8-phenyl- (9CI) (CA INDEX NAME)

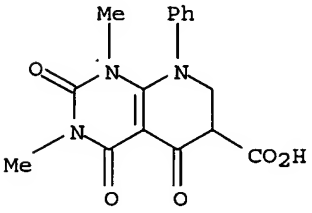


RN 171507-52-1 HCAPLUS

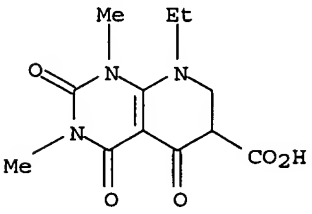
CN Pyrido[2,3-d]pyrimidine-6-carboxamide, 8-ethyl-1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo- (9CI) (CA INDEX NAME)



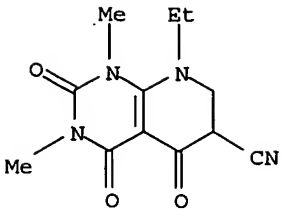
IT **171507-55-4P 171507-57-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)
RN 171507-55-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo-8-phenyl- (9CI) (CA INDEX NAME)



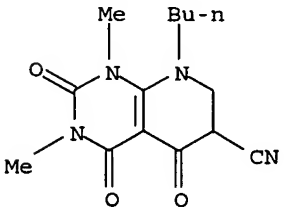
RN 171507-57-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 8-ethyl-1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo- (9CI) (CA INDEX NAME)



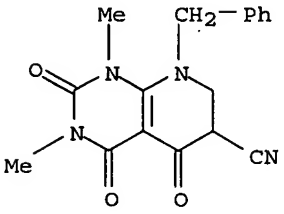
IT **171507-44-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)
RN 171507-44-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carbonitrile, 8-ethyl-1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo- (9CI) (CA INDEX NAME)



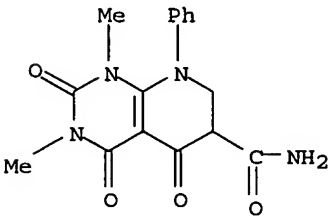
IT 171507-45-2P 171507-47-4P 171507-53-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, hydrolysis, and bactericidal activity of cyanopyridopyrimidinetriones)
RN 171507-45-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carbonitrile, 8-butyl-1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo- (9CI) (CA INDEX NAME)



RN 171507-47-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carbonitrile, 1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo-8-(phenylmethyl)- (9CI) (CA INDEX NAME)



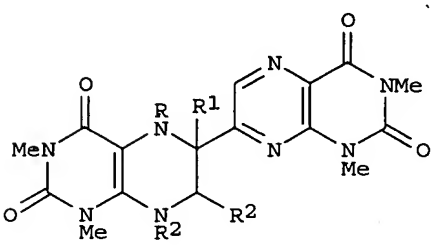
RN 171507-53-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxamide, 1,2,3,4,5,6,7,8-octahydro-1,3-dimethyl-2,4,5-trioxo-8-phenyl- (9CI) (CA INDEX NAME)



L38 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:394467 HCAPLUS
DN 122:214436
ED Entered STN: 04 Mar 1995

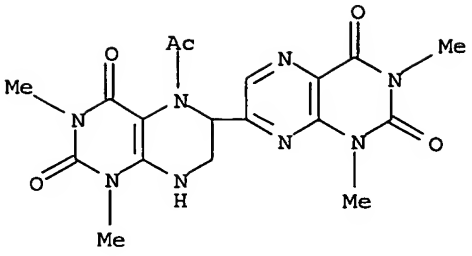
Search done by Noble Jarrell

TI Pteridines CII. Synthesis and characterization of dimeric lumazines
AU Koul, Ashok; Wagner, Thomas; Pfleiderer, Wolfgang
CS Fakultaet Chemie, Univ. Konstanz, Konstanz, D-78434, Germany
SO Pteridines (1994), 5(4), 121-8
CODEN: PTRDEO; ISSN: 0933-4807
PB International Society of Pteridinology
DT Journal
LA English
CC 33-9 (Carbohydrates)
GI

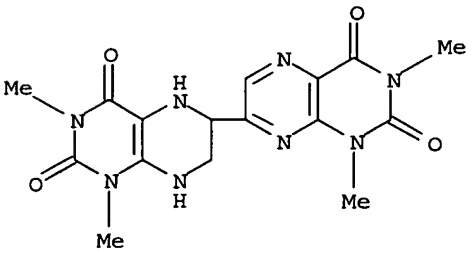


I

AB Reduction of 1,3-dimethyllumazine by zinc dust in Ac2O/AcOH leads to the formation of 6-7 connected bis-lumazinyl derivs. Depending on the reaction conditions either 7-(5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazin-6-yl)-1,3-dimethyllumazin I, (R = Ac, R1 = R2 = H) or isomeric 7-(5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazin-6-yl)-5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazines (II) are formed. Treatment of I (R = Ac, R1 = R2 = H) with MeOH/HCl gave I (R = R1 = R2 = H) which is oxidized by air to a very stable 7,8-dihydro derivative I (RR1 = bond, R2 = H) showing unexpected spectra properties. Further oxidation by KMnO4 afforded 6,7-bis-1,3-dimethyllumazinyl I (RR1 = bond, R22 = bond). Isomeric 6,6- and 7,7-bis-1,3-dimethyllumazinyls were also synthesized from 6-chloro- and 7-chloro-1,3-dimethyllumazine, resp., in a nickel catalyzed dimerization reaction. The various structures were proven by spectral means, elemental analyses and an x-ray anal. of II. Comparisons of the structural features are mainly based on UV data.
ST lumazine dimeric
IT 84689-47-4, 6-Chloro-1,3-dimethyllumazine 84689-48-5, 6-Bromo-1,3-dimethyllumazine 84689-49-6, 7-Chloro-1,3-dimethyllumazine 84689-50-9, 2,4(1H,3H)-Pteridinedione, 7-bromo-1,3-dimethyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dimeric lumazines)
IT 13401-18-8P, 1,3-Dimethyllumazine **161959-61-1P** **161959-62-2P** 161959-63-3P 161959-66-6P 161959-68-8P 161959-71-3P 161959-73-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dimeric lumazines)
IT **161959-60-0P** 161959-64-4P **161959-65-5P** 161959-67-7P **161959-69-9P** **161959-70-2P** 161959-72-4P 161959-74-6P 161959-75-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dimeric lumazines)
IT **161959-61-1P** **161959-62-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dimeric lumazines)
RN 161959-61-1 HCAPLUS
CN [6,7'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5-acetyl-5,6,7,8-tetrahydro-1,1',3,3'-tetramethyl- (9CI) (CA INDEX NAME)

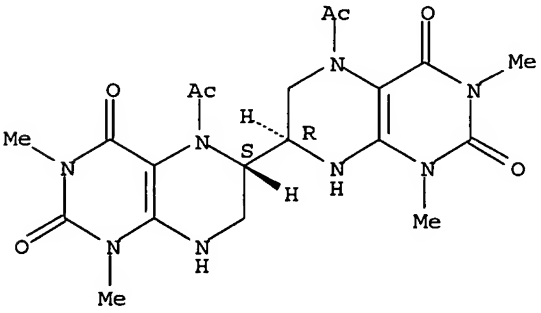


RN 161959-62-2 HCAPLUS
CN [6,7'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5,6,7,8-tetrahydro-1,1',3,3'-tetramethyl- (9CI) (CA INDEX NAME)



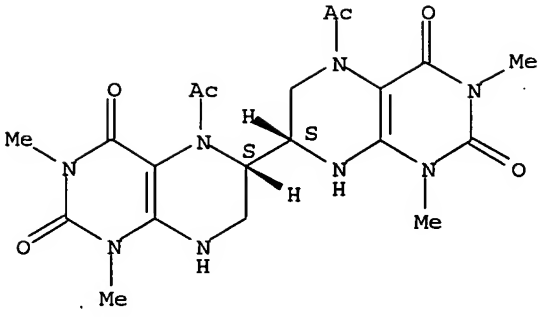
IT **161959-60-0P 161959-65-5P 161959-69-9P 161959-70-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dimeric lumazines)
RN 161959-60-0 HCAPLUS
CN [6,7'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5,5'-diacetyl-5,5',6,6',7,7',8,8'-octahydro-1,1',3,3'-tetramethyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

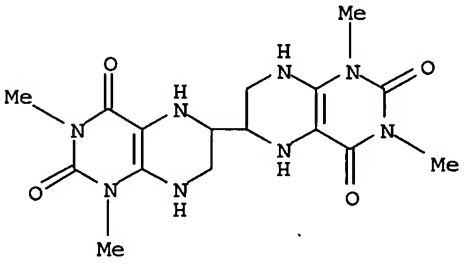


RN 161959-65-5 HCAPLUS
CN [6,7'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5,5'-diacetyl-5,5',6,6',7,7',8,8'-octahydro-1,1',3,3'-tetramethyl-, (R*,R*)- (9CI) (CA INDEX NAME)

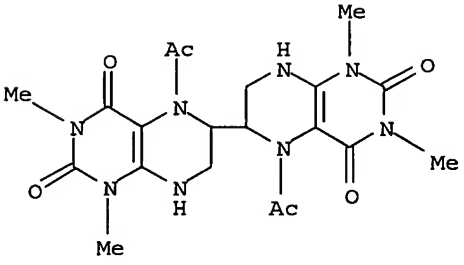
Relative stereochemistry.



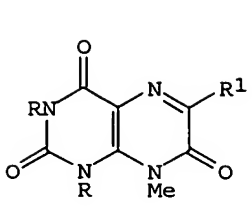
RN 161959-69-9 HCAPLUS
CN [6,6'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5,5',6,6',7,7',8,8'-octahydro-1,1',3,3'-tetramethyl- (9CI) (CA INDEX NAME)

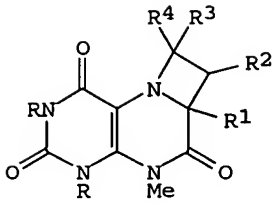


RN 161959-70-2 HCAPLUS
CN [6,6'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 5,5'-diacetyl-5,5',6,6',7,7',8,8'-octahydro-1,1',3,3'-tetramethyl- (9CI) (CA INDEX NAME)



L38 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:221670 HCAPLUS
DN 108:221670
ED Entered STN: 24 Jun 1988
TI Photochemical [2+s2] cycloadditions of the C = N bond of pteridine-2,4,7-triones to alkenes
AU Nishio, Takehiko; Nishiyama, Tadashi; Omote, Yoshimori
CS Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Liebigs Annalen der Chemie (1988), (5), 441-3
CODEN: LACHDL; ISSN: 0170-2041
DT Journal
LA English
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 108:221670
GI


I


II

AB Irradiation of pteridine-2,4,7-triones I (R = Me, Ph; R1 = Me) in the presence of electron-deficient and neutral alkenes, R2CH:CR3R4 (R2 = H, cyano, Ph, CO2Me; R3 = H, Me, Ph; R4 = cyano, CO2Me, Ph) gave azetidines II via [2 + 2] cycloaddn. reaction of the C=N double bond of I to the alkenes in a regiospecific manner. Irradiation of I (R = Me, Ph; R1 = Ph) did not give photocycloadduct with methacrylonitrile.

ST pteridinetrione alkene cycloaddn photochem regiochem

IT Regiochemistry
(of photochem. cycloaddn. of pteridinetriones to electron-deficient alkenes)

IT Cycloaddition reaction
([2+2], photochem., of pteridinetriones to electron-deficient alkenes, azetidines from)

IT 109-92-2, Ethyl vinyl ether 110-83-8, Cyclohexene, reactions 115-11-7, Isobutene, reactions 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted photochem. cycloaddn. of, with pteridinetriones)

IT 80-62-6, Methyl methacrylate 107-13-1, Acrylonitrile, reactions 126-98-7, Methacrylonitrile 530-48-3, 1,1-Diphenylethylene 624-49-7, Dimethyl fumarate 764-42-1, Fumaronitrile 4360-47-8, Cinnamonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn. of, with pteridinetriones)

IT 109853-23-8P 113088-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and attempted photochem. cycloaddn. of, with methacrylonitrile)

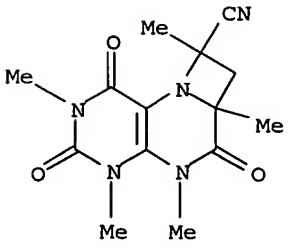
IT 99069-70-2P 113088-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cycloaddn. of, azetidines from)

IT **113088-56-5P 113088-57-6P 113088-58-7P**
113088-59-8P 113088-60-1P 113088-61-2P
113088-62-3P 113088-63-4P 113088-64-5P
113088-65-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **113088-56-5P 113088-57-6P 113088-58-7P**
113088-59-8P 113088-60-1P 113088-61-2P
113088-62-3P 113088-63-4P 113088-64-5P
113088-65-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

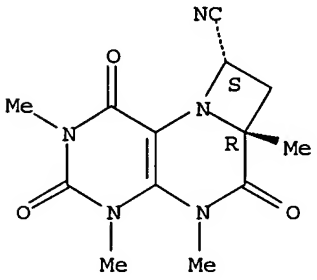
RN 113088-56-5 HCAPLUS

CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a,8-pentamethyl-1,3,6-trioxo- (9CI) (CA INDEX NAME)



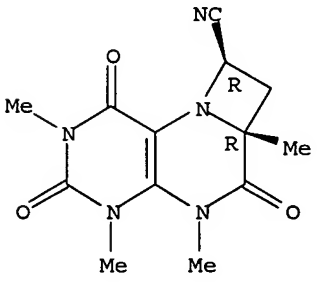
RN 113088-57-6 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a-tetramethyl-1,3,6-trioxo-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

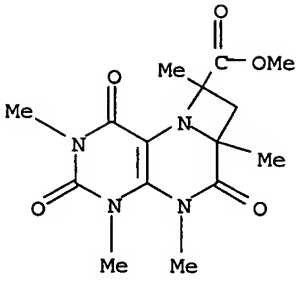


RN 113088-58-7 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a-tetramethyl-1,3,6-trioxo-, cis- (9CI) (CA INDEX NAME)

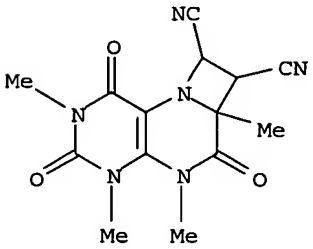
Relative stereochemistry.



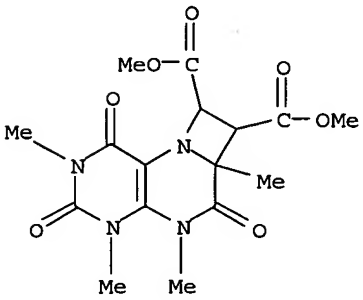
RN 113088-59-8 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carboxylic acid, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a,8-pentamethyl-1,3,6-trioxo-, methyl ester (9CI) (CA INDEX NAME)



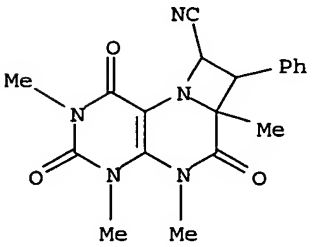
RN 113088-60-1 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-7,8-dicarbonitrile, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a-tetramethyl-1,3,6-trioxo- (9CI) (CA INDEX NAME)



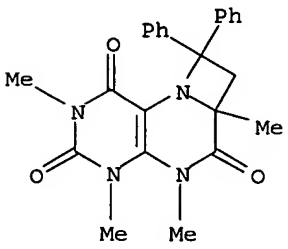
RN 113088-61-2 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-7,8-dicarboxylic acid, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a-tetramethyl-1,3,6-trioxo-, dimethyl ester (9CI) (CA INDEX NAME)



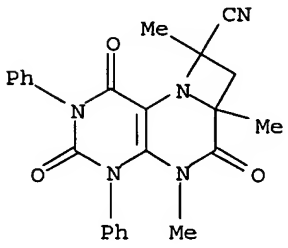
RN 113088-62-3 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-2,4,5,6a-tetramethyl-1,3,6-trioxo-7-phenyl- (9CI) (CA INDEX NAME)



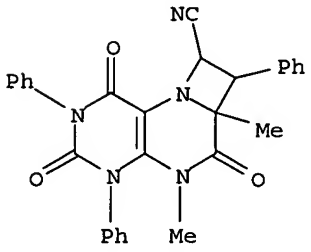
RN 113088-63-4 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-1,3,6(4H,5H,6aH)-trione, 7,8-dihydro-2,4,5,6a-tetramethyl-8,8-diphenyl- (9CI) (CA INDEX NAME)



RN 113088-64-5 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-5,6a,8-trimethyl-1,3,6-trioxo-2,4-diphenyl- (9CI) (CA INDEX NAME)

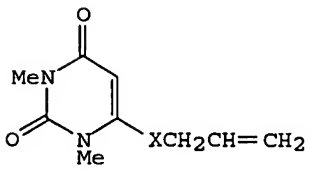


RN 113088-65-6 HCAPLUS
CN 2H-Azeto[1,2-f]pteridine-8-carbonitrile, 1,3,4,5,6,6a,7,8-octahydro-5,6a-dimethyl-1,3,6-trioxo-2,4,7-triphenyl- (9CI) (CA INDEX NAME)

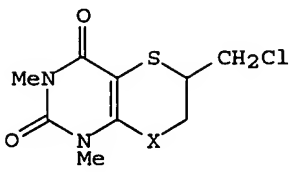


L38 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:18476 HCAPLUS
DN 106:18476
ED Entered STN: 24 Jan 1987
TI Studies on pyrimidine annelated heterocycles: cyclization of 1,3-dimethyluracil-6-allyl ether and its analogs with sulfur dichloride
AU Bhuyan, Pulak J.; Boruah, Romesh C.; Sandhu, Jagir S.
CS Div. Drugs Pharm., Reg. Res. Lab., Jorhat, 785 006, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(11), 1166-7
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 106:18476
GI

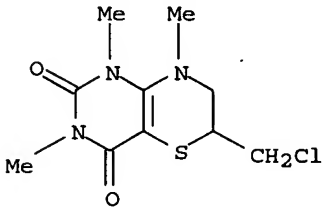


I

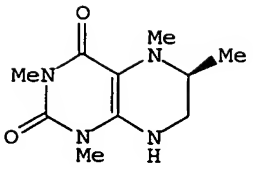


II

AB SCl2 reacts with 1,3-dimethyluracil derivs. I (X = O, S, NMe) to afford annulated pyrimidine derivs. II.
ST pyrimidooxathiin; pyrimidodithiin; pyrimidothiazine
IT 105459-34-5P 105459-35-6P **105803-17-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 93767-20-5 105459-36-7 105459-37-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfur dichloride)
IT **105803-17-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 105803-17-6 HCAPLUS
CN 1H-Pyrimido[5,4-b][1,4]thiazine-2,4(3H,6H)-dione, 6-(chloromethyl)-7,8-dihydro-1,3,8-trimethyl- (9CI) (CA INDEX NAME)



L38 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:121469 HCAPLUS
DN 94:121469
ED Entered STN: 12 May 1984
TI Studies on biologically active pteridines. V. Synthesis of (6S)-5,6,7,8-tetrahydro-1,3,5,6-tetramethyllumazine
AU Sugimoto, Takashi; Matsuura, Sadao
CS Coll. Gen. Educ., Nagoya Univ., Nagoya, 464, Japan
SO Bulletin of the Chemical Society of Japan (1980), 53(11), 3385-6
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA English
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
GI



I

AB (+)-5,6,7,8-Tetrahydro-1,3,5,6-tetramethyllumazine (I) a compound derived from enzymically reduced (-)-5,6,7,8-tetrahydro-6-methylpterin, was shown to be of (S)-configuration at the C-6 chiral center by a synthesis, which was performed by condensation of 5-bromo-6-chloro-1,3-dimethyluracil with (2S)-1-amino-2-(methylamino)propane. The structure of the condensation product was determined unequivocally by an independent synthesis using a regioselective methylation of 5,6,7,8-tetrahydro-1,3,6-trimethyllumazine.

ST lumazine tetrahydro tetramethyl

IT 21428-25-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with amino(methylamino)propane, tetrahydrotetramethyllumazine from)

IT 7324-05-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)

IT 14006-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation and methylation of)

IT 27255-44-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclization with bromochlorodimethyluracil)

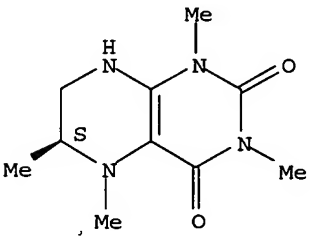
IT **76909-38-1P 76946-49-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **76909-38-1P 76946-49-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 76909-38-1 HCAPLUS

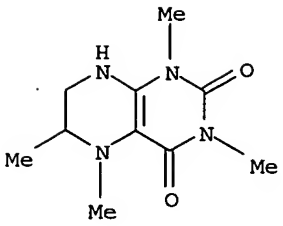
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3,5,6-tetramethyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

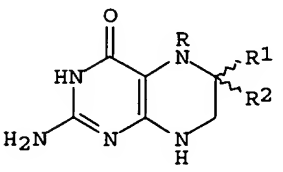


RN 76946-49-1 HCAPLUS

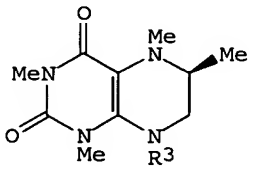
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)



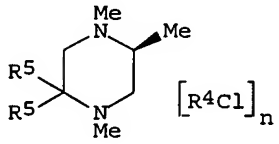
L38 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1980:550214 HCAPLUS
DN 93:150214
ED Entered STN: 12 May 1984
TI Absolute configuration of 6-methyl-5,6,7,8-tetrahydropterin produced by enzymic reduction (dihydrofolate reductase and NADPH) of 6-methyl-7,8-dihydropterin
AU Armarego, Wilfred L. F.; Waring, Paul; Williams, Jeffrey W.
CS John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, 2601, Australia
SO Journal of the Chemical Society, Chemical Communications (1980), (8), 334-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 7, 22
GI



I



III

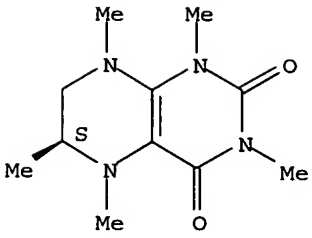


IV

AB The absolute configuration of enzymically prepared 6-methyl-5,6,7,8-tetrahydropterin (I; R = H, R1 = α-H, R2 = β-Me) (II) was confirmed by correlation with (S)-alanine, by a series of methylations and degrdns. Thus, reduction of I (RR1 = bond, R2 = Me) with dihydrofolate reductase and NADPH gave (-)-II. Treatment of (-)-II.HCl with MeI and NaOH in MeOH, followed by deamination, gave (+)-III.HCl (R3 = H). This was methylated to (+)-III (R3 = Me) and degraded to an intermediate piperazinone, which was methylated and acidified with 2N HCl to give (+)-IV (R4 = Me, R52 = O, n = 1). (+)-IV (R4 = R5 = H, n = 2) was prepared from glycyl-(S)-alanine via the known (S)-(-)-3-methylpiperazine-2,5-dione, and thus the stereochem. of II was confirmed.
ST configuration abs enzymically produced methylpterin; pterin methyl abs configuration; stereochem redn enzymic methylpterin
IT Reduction
(of methyldihydropterin by dihydrofolate reductase, stereochem. of)
IT Stereochemistry
(of reduction of methyldihydropterin by dihydrofolate reductase)

IT Configuration
(absolute, of methyltetrahydropterin, enzymically produced)
IT 78-98-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with glycine methylamide)
IT 22356-89-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with pyruvaldehyde)
IT 73573-51-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(enzymic preparation and absolute configuration of)
IT 17377-13-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(enzymic reduction of)
IT 74893-13-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deamination of)
IT **74879-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and degradation of)
IT 74879-14-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 74879-09-7P **74879-10-0P** 74879-13-3P 74879-18-8P
74923-39-0P 74923-44-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
IT 74879-15-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with dibenzoyltartaric acid)
IT 4526-77-6P 74879-12-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 74923-41-4P 74923-43-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and resolution of)
IT 74879-17-7P 74893-14-4P 74923-45-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 53-57-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by dihydrofolate reductase and, of methyldihydropterin)
IT 9002-03-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of methyldihydropterin)
IT 3695-73-6
RL: PROC (Process)
(sublimation of, methylpiperazinedione by)
IT **74879-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and degradation of)
RN 74879-11-1 HCAPLUS
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3,5,6,8-pentamethyl-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

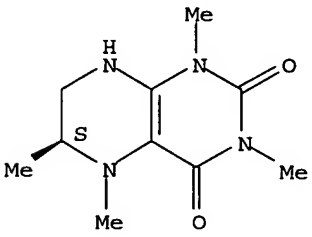
Absolute stereochemistry.



● HCl

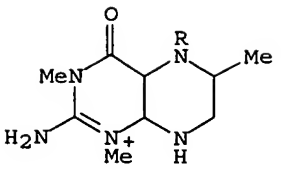
IT 74879-10-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 74879-10-0 HCAPLUS
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3,5,6-tetramethyl-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L38 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1978:509374 HCAPLUS
DN 89:109374
ED Entered STN: 12 May 1984
TI Pterins. III. Methylation of 6-methyl-5,6,7,8-tetrahydropterin, N-5-demethylation of 1,3,5,6-tetramethyl-5,6,7,8-tetrahydropterinium chloride hydrochloride and exchange of the 5-methyl group in 5,6-dimethyl-5,6,7,8-tetrahydropterin
AU Armarego, Wilfred L. F.; Schou, Henning
CS John Curtin Sch. Med. Res., Australian Natl. Univ., Canberra, Australia
SO Australian Journal of Chemistry (1978), 31(5), 1081-94
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22, 7
GI



Cl^- I, R=H
II, R=Me

AB Methylation of 6-methyl-5,6,7,8-tetrahydropterin in the presence of NaOH furnishes 1,3,6-trimethyl-5,6,7,8-tetrahydropterinium chloride (I) which can be methylated further to yield 1,3,5,6-tetramethyl-5,6,7,8-tetrahydropterinium chloride (II). Demethylation of II occurred on a Dowex 50W/3N-aqueous NH3 column with loss of the 5-Me group to give I. The structures of these salts were deduced by a study of similar alkylations of authentic 1,6-dimethyl-, 3,6-dimethyl-, 5,6-dimethyl-, 6,8-dimethyl-, 1,5,6-trimethyl-, and 3,5,6-trimethyl-5,6,7,8-tetrahydropterin, and of 6-methyl-2-methylamino-5,6,7,8-tetrahydropteridin-4(3H)-one. Methylation of 5,6-dimethyl-5,6,7,8-tetrahydropterin, with D3CI in the presence of alkali gave II in which considerable exchange of the 5-Me group by a trideuteromethyl group had taken place. I and II were considerably more stable to aerial oxidation than 6-methyl-, 1,6-, 3,6-, 5,6-, 6,7-, 6,8-dimethyl-, and 1,5,6-trimethyl-5,6,7,8-tetrahydropterins. Loss of the 5-Me group from II, and exchange of the 5-Me group in 5,6-dimethyl-5,6,7,8-tetrapterin, allowed a mechanism for the enzymic transfer of the 5-Me group in 5-methyl-5,6,7,8-tetrahydrofolic acid in biol. methylations to be proposed.

ST methylation methyltetrahydropterin; pterin methyl tetrahydro methylation; demethylation tetramethyltetrahydropterinium; oxidn tetramethyltetrahydropterinium; enzyme methyl transfer mechanism

IT Methylation
(of methyltetrahydropterin)

IT Oxidation
(of methyltetrahydropteriniums and methyltetrahydropterins)

IT Kinetics of oxidation
(of methyltetrahydropterins)

IT Demethylation
(of tetramethyltetrahydropterinium chloride hydrochloride)

IT 67129-04-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)

IT 69113-63-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(neutralization and methylation of)

IT 611-54-1 942-41-6 20041-70-7 25239-84-3 67129-02-6 67129-03-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, kinetics of)

IT 67128-91-0P 67128-92-1P 67128-93-2P 67128-95-4P 67128-96-5P 67128-97-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

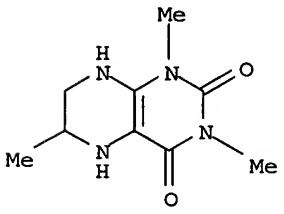
IT 3116-65-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 67128-94-3P 67129-00-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 67128-99-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, demethylation, and oxidation of)

IT 67128-98-7P

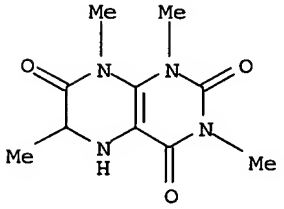
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, methylation, and oxidation of)
IT 67129-05-9 67194-33-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT **67128-94-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 67128-94-3 HCAPLUS
CN 2,4(1H,3H)-Pteridinedione, 5,6,7,8-tetrahydro-1,3,6-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



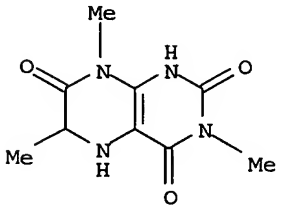
●x HCl

L38 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1965:443426 HCAPLUS
DN 63:43426
OREF 63:7781h,7782a-b
ED Entered STN: 22 Apr 2001
TI Electron spectroscopic determination of the directions of transition and of the ionization and tautomerism constants of 7-hydroxylumazine and of its methyl derivatives
AU Prigge, H.; Lippert, E.
CS Tech. Hochsch., Stuttgart, Germany
SO Berichte der Bunsen-Gesellschaft (1965), 69(6), 458-67
CODEN: BBPCAX; ISSN: 0940-483X
DT Journal
LA German
CC 10 (Spectra and Some Other Optical Properties)
GI For diagram(s), see printed CA Issue.
AB The uv absorption and fluorescence spectra are investigated in different media. The ionization constants of the compounds investigated are determined from the pH dependence of the absorption spectra. The 7-hydroxylumazines (I) exist in tetrahydrofuran in their enolic form (II). In aqueous solution a (7-OH enol)/(8-H amide) tautomerism exists. The consts. of tautomerism, KT = [8-H]/[7-OH], depend on the number and position of the Me substituents. A Me group at the 1-N atom hinders sterically the amide form, while a Me group at the 6-C atom hinders the enolic form. The spectra are discussed, considering the structures of the neutral mols., the cations and the anions, as well as the direction of polarization of the $\pi \rightarrow \pi^*$ electronic transitions, and this also by means of the absorption polarization spectra of its fluorescence.
IT aci-Nitro compounds
(mol. orbitals and spectra of)
IT Ionization
(of 7-hydroxylumazine and its Me derivs.)
IT Fluorescence
Spectra, visible and ultraviolet
(of 7-hydroxylumazine and its Me derivs., ionization and tautomerism in relation to)
IT Substituents

(tautomerism and, of 7-hydroxylumazine derivs.)
IT Isomerism, Isomers
(tautomerism, of 7-hydroxylumazine and its Me derivs.)
IT Butane, 2-methyl-3-aci-nitro-
Propane, 2-methyl-1-aci-nitro-
(sodium derivative, spectrum of)
IT 2614-42-8, Lumazine, 7-methoxy-1,3-dimethyl- 2614-43-9, Lumazine, 7-hydroxy-1,3-dimethyl- 2614-44-0, Lumazine, 7-hydroxy-1-methyl- 2622-65-3, Lumazine, 7-hydroxy-3-methyl- 2622-66-4, Lumazine, 7-methoxy-1,3,6-trimethyl- 2625-21-0, Lumazine, 7-hydroxy-1,3,6-trimethyl- 2625-22-1, Lumazine, 7-hydroxy-1,6-dimethyl- 2625-23-2, Lumazine, 7-hydroxy-3,6-dimethyl- 2625-25-4, Lumazine, 1,3,6,7-tetramethyl- **3215-22-3**, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3,6,8-tetramethyl- **3215-23-4**, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-3,6,8-trimethyl- 3220-42-6, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-3,8-dimethyl- 3220-43-7, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-8-methyl- 31053-46-0, Lumazine, 7-hydroxy-6-methyl- 90971-99-6, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3,8-trimethyl-
(fluorescence and spectrum of, ionization and tautomerism in relation to)
IT 2577-38-0, Lumazine, 7-hydroxy-
(fluorescence and spectrum of, ionization and tautomersim in relation to)
IT **3215-22-3**, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3,6,8-tetramethyl- **3215-23-4**, 2,4,7-(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-3,6,8-trimethyl-
(fluorescence and spectrum of, ionization and tautomerism in relation to)
RN 3215-22-3 HCAPLUS
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3,6,8-tetramethyl- (7CI, 8CI) (CA INDEX NAME)



RN 3215-23-4 HCAPLUS
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-3,6,8-trimethyl- (7CI, 8CI) (CA INDEX NAME)



L38 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1964:440466 HCAPLUS
DN 61:40466
OREF 61:7025b-e
ED Entered STN: 22 Apr 2001
TI Pyrazolo[3,4-d]pyrimidines

PA CIBA Ltd.
SO 6 pp.
DT Patent
LA Unavailable
IC C07D
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GB 937725		19630925	GB	<--
PRAI CH		19600511 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
GB 937725	IC	C07D

GI For diagram(s), see printed CA Issue.
AB The title compds. (I) were prepared by treating I with N2H4, NH3, or an aliphatic amine. A mixture of 15 g. 1-phenyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine and 100 ml. POCl3 was refluxed for 6 hrs. Excess POCl3 was evaporated, the residue dissolved in CHCl3 and extracted with H2O and NaHCO3 solution The CHCl3 was then evaporated to give I (R = Ph, R1 = H, R2 = Cl, R3 = benzyl) (II), m. 90-1° (CHCl3-ligroine). II (7 g.) and 25 g. Me2NH in 50 ml. EtOH were heated in an autoclave for 7 hrs. at 100° to give I (R = Ph, R1 = H, R2 = Me2N, R3 = benzyl), m. 121-2° (EtOH). Similarly prepared were the following I (R, R1, R2, R3, recrystallization solvent, and m.p. given): iso-Pr, H, Me2N, benzyl, ligroine, 117-18°; iso-Pr, H, H2NNH, benzyl, EtOH, 136-7°; Ph, H, piperidino, benzyl, EtOH, 116-18°; Ph, H, 4-methyl-1-piperazinyl, benzyl, EtOH, 122°; iso-Pr, H, piperidino, Ph, ligroine, 127.5-8.5°; iso-Pr, H, Et2N, Ph, Et2O, 104-5°. Prepared similarly to II was I (R = iso-Pr, R1 = H, R2 = Cl, R3 = Ph), m. 106-7°. A ground mixture of 2-isopropyl-3-aminopyrazole-4-carboxamide and benzamide was heated for 10 hrs. at 270°. The mixture was dissolved in 2N NaOH, filtered and the filtrate brought to pH 6 with 5N HCl to give I (R = iso-Pr, R1 = H, R2 = OH, R3 = Ph), m. 256-8° (EtOH). I are useful as coronary dilators.
IT Blood vessels
(dilators of, 1H-pyrazolo[3,4-d]pyrimidines as)
IT 271-80-7, 1H-Pyrazolo[3,4-d]pyrimidine
(derivs.)
IT 92165-44-1, 1H-Pyrazolo[3,4-d]pyrimidine, 4-chloro-1-isopropyl-6-phenyl- 92193-22-1, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-phenyl- 92871-93-7, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-hydrazino-1-isopropyl- 94030-23-6, 1H-Pyrazolo[3,4-d]pyrimidine, 4-(diethylamino)-1-isopropyl-6-phenyl- 94548-52-4, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-(dimethylamino)-1-phenyl- 94916-12-8, 1H-Pyrazolo[3,4-d]pyrimidine, 1-isopropyl-6-phenyl-4-piperidino- 94994-79-3, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-chloro-1-phenyl- 96267-34-4, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-(4-methyl-1-piperazinyl)-1-phenyl- 96368-88-6, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-phenyl-4-piperidino- 98132-44-6, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-(dimethylamino)-1-isopropyl-
(preparation of)

L38 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1964:440465 HCAPLUS
DN 61:40465
OREF 61:**7024h,7025a-b**
ED Entered STN: 22 Apr 2001
TI Pyrido[2,3-d]pyrimidine-2,4,5,7-tetraones
IN Scarborough, Homer C.
PA Mead Johnson & Co.
SO 2 pp.
DT Patent
LA Unavailable
INCL 260256400
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3139432		19640630	US	19630624 <--
	GB 989048			GB	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3139432	INCL	260256400
US 3139432	NCL	544/279.000 <--

GI For diagram(s), see printed CA Issue.

AB Malonic acids are condensed with a 4-aminouracil in the presence of an acid anhydride to give compds. of the general formula I which can be used as bronchodilators. A mixture of 8.45 g. 1,3-dimethyl-4-(methylamino)uracil, 7.1 g. MeCH(CO2H)2, 11.3 ml. Ac2O, and 10 ml. HOAc is heated 2 hrs. on a steam bath, cooled, and filtered to give 48% 1,3,6,8-tetramethylpyrido[2,3-d]-pyrimidine-2,4,5,7-[1H,3H,6H,8H]-tetraone, m. 259.5-60.5° (MeCN). Similarly prepared are I(R = R1 = R2 = R3 = H),m. >360°; and the following I(R = R1 = Me)(R2,R3,and m.p. given): H, H, 280-2.5°; H, Me, 220.5-2.5°; Me, H, 287-9.5°; Bu, H, 195-6°; Bu, Me, 119-20°. Also prepared is the Na salt of I (R2 = H, R = R1 = R3 = Me).

IT Bronchi
(dilating substances for, pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrones as)

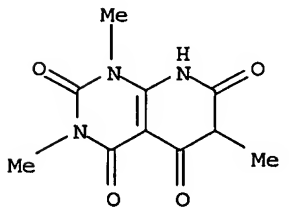
IT 271-80-7, 1H-Pyrazolo[3,4-d]pyrimidine 91996-75-7, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone
(derivs.)

IT 91996-75-7, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone 93117-35-2, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3-dimethyl- 93117-36-3, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3-dimethyl- 93738-66-0, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,8-trimethyl- 93738-67-1, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6-trimethyl- 93738-68-2, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,8-trimethyl- **93738-69-3**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6-trimethyl- **95709-04-9**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6,8-tetramethyl- **96732-25-1**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3-dimethyl- 96986-13-9, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3-dimethyl- 97360-49-1, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl- **97864-53-4**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3,8-trimethyl-
(preparation of)

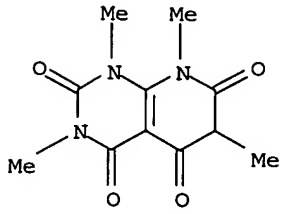
IT **93738-69-3**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6-trimethyl- **95709-04-9**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6,8-tetramethyl- **96732-25-1**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3-dimethyl- **97864-53-4**, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3,8-trimethyl-
(preparation of)

RN 93738-69-3 HCAPLUS

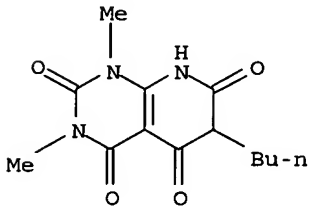
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6-trimethyl- (7CI) (CA INDEX NAME)



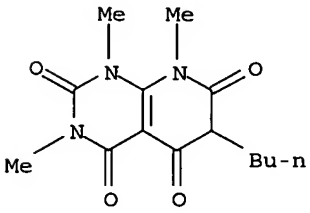
RN 95709-04-9 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6,8-tetramethyl- (7CI) (CA INDEX NAME)



RN 96732-25-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3-dimethyl- (7CI) (CA INDEX NAME)



RN 97864-53-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3,8-trimethyl- (7CI) (CA INDEX NAME)



L38 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1964:440464 HCAPLUS
DN 61:40464
OREF 61:**7024f-h**
ED Entered STN: 22 Apr 2001
TI Tetrahydropyrimidinone
IN Boswell, George A.; Williams, Paul H.
PA Shell Oil Co.
SO 4 pp.
DT Patent
LA Unavailable
INCL 260251000
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3137697		19640616	US	19620319 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3137697	INCL	260251000

US 3137697 NCL 544/315.000; 544/318.000; 564/048.000; 564/052.000; 564/057.000; 564/058.000; 564/059.000; 564/060.000 <--

GI For diagram(s), see printed CA Issue.

AB Urea (120 g.) in iso-PrOH at 70° was treated dropwise with 147 cc. 93% acrolein, 90% of the acrolein was consumed in 30 hrs., and 1100 cc. of the reaction mixture was hydrogenated in the presence of 10-15 moles NH3 [to produce 1-(3-aminopropyl)urea] per mole of acrolein at 150° and 1500 lb./in.2 over 40 g. Raney Ni to yield 50 g. I, m. 250-5°. I and HCHO gave the 1,3-dimethylol derivative, m. 245-50°, which imparts crease-resistant properties to textiles.

IT 1852-17-1, 2(1H)-Pyrimidinone, tetrahydro-
(manufacture of)

L38 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:435664 HCAPLUS

DN 59:35664

OREF 59:6420h,6421a-g

ED Entered STN: 22 Apr 2001

TI 3,6,8-Trioxopyrimido[5,4-b]-1,4-thiazines

IN Schroeder, Elmer F.

PA G.D. Searle and Co.

SO 5 pp.

DT Patent

LA Unavailable

INCL 260243000

CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3080364		19630305	US	19610526 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3080364	INCL	260243000
US 3080364	NCL	544/048.000; 504/221.000; 544/311.000 <--

GI For diagram(s), see printed CA Issue.

AB Thioglycolic acid (I) 6.07 in H2O 25 heated 0.5 hr. at 100° with 1-propyl-3-ethyl-5-chloro-6-aminouracil 13.9 in NaOH 2.4 and H2O 35 parts gave 1-propyl-3-ethyl-5-carboxymethylthio-6-aminouracil (II), m. 182-4°. I 6.07 in H2O 25 similarly treated with 1,3-dimethyl-5-chloro-6-aminouracil 11.37 parts gave 1,3-dimethyl-5-carboxymethylthio-6-aminouracil (III), m. 218-20° (effervescence). 1-Allyl-3-ethyl-5-chloro-6-aminouracil similarly treated with I in alkali gave 1-allyl-3-ethyl-5-chloro-6-aminouracil (IV), m. 176-7°. I and 1,3-dibutyl-5-chloro-6-aminouracil gave 1,3-dibutyl-5-carboxymethylthio-6-aminouracil (V), m. 157-9°. 1-(2-Hydroxyethyl)-3-ethyl-5-chloro-6-aminouracil and I similarly gave 1-(2-hydroxyethyl)-3-ethyl-5-carboxymethylthio-6-aminouracil (VI), m. 206-7°. III 12.3 refluxed 5 min. with Ac2O 43.5 parts gave 5,7-dimethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (VII), m. 270-2° (darkening at 260°). II similarly treated with Ac2O gave 5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (VIII), m. 186-8°. V and Ac2O gave 5,7-dibutyl-3,6,8-trioxopyrimido [5,4-b]-1,4-thiazine (IX), m. 213-14°. IV and Ac2O also gave 5-allyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine, m. 231-3°. VI and Ac2O gave 5-(2-hydroxyethyl)-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (IX), m. 225-6°. VIII 11 in CHCl3 180 kept 1 hr. at 5-10° with BzOOH 6 in C6H6 108 gave 5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine 1-oxide (X), m. 165-7° (decomposition). VII similarly afforded the corresponding 1-oxide (XI). VIII 13, NaHCO3 5, and anhydrous CHCl3 186 treated slowly with Br 8 in CHCl3 75 parts, stirred 15 min. at 10-15°, and the product separated gave 2-bromo derivative (XIa), m. 197-9° (decomposition). VII similarly afforded 2-bromo derivative VIII 16.2 suspended in AcOH 94.5 treated with sulfuryl chloride 8.1 parts, kept 0.5 hr. at room temperature, and the product separated gave 2-chloro derivative (XII), m. 203-5° (decomposition). X 20 and AcOH 82 parts heated several min. gave 2-acetoxy-5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4b]-1,4-thiazine (XIII),

m. 159-60° (effervescence). XIa 35, NaOAc 82, and AcOH 200 parts heated a few min. on the steam bath gave XIII. XI similarly gave 2-acetoxy-5,7-dimethyl- 3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine. Similar treatment of XI with EtCO2H gave 2-propionyloxy-5,7-dimethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine and X gave 2-propionyloxy-5 propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine. X 5 in MeOH 48 parts refluxed a few min. gave 2-methoxy-5-propyl-7-ethyl-3,6,8-trioxopyrimido [5,4-b]-1,4-thiazine, m. 199-200° (decomposition). X 10 in EtOH 115 parts refluxed several min., treated with C, and cooled gave 2-ethoxy-5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (XIV), m. 163-5°. XIa similarly treated with alc. gave XIV. VIII 27, CCl4 460, and sulfuryl chloride 27 parts refluxed 1.5 hrs. gave 2,2-dichloro derivative (XV), m. 145-7°. XV 7 in MeOH 28 parts kept 1 hr. at room temperature gave 2,2-dimethoxy analog, m. 162-3°. XIV 16 and AcOH 60 treated 0.5 hr. at room temperature with 40% AcOOH 10 parts gave the 1-oxide (XVI), m. 185-7°. XVI in EtOH refluxed 4 hrs. gave 2,2-diethoxy-5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (XVII), m. 165-7°. XV similarly treated with EtOH gave XVII. 2-Ethoxy-5,7-dimethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine similarly treated gave 2,2-diethoxy derivative VII 4.55 suspended in AcOH 52.5 kept 0.5 hr. with sulfuryl chloride 2.7 parts gave 2-chloro derivative (XVIII), m. 335-7° (decomposition). XVIII in EtOH refluxed 10 min. gave 2-ethoxy analog (XIX), m. 217-19° (decomposition). 2-Chloro-5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (XX) 6.08 and BuOH 25 parts heated 3 min. at 100° gave 2-butoxy analog, m. 136-7°. Similarly, XX treated with 2-chloroethanol gave 2-(2-chloroethoxy) analog, m. 158-9°. X kept 48 hrs. in H2O at room temperature gave 2-hydroxy-5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine (XXI), m. 205-7° (decomposition). XIII refluxed 15 min. with H2O gave XXI. 1-Propyl-3-ethyl-5-carboxymethylsulfonyl-6-aminouracil 9.5 and Ac2O 20.5 parts heated 4 hrs. at 100° gave 5-propyl-7-ethyl-3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine 1,1-dioxide, m. 248-9°. 6-Aminouracil 6.35 in HCONMe2 60.3 treated over 1 hr. at room temperature with sulfuryl chloride 6.75 parts, then stirred 2 hrs., and the product precipitated gave 6-amino-6-chlorouracil (XXII), darkens about 325°. XXII 16.1 in H2O 60 containing NaOH 9 heated 45 min. at 100° with I 10.2 parts gave 6-amino-5-carboxymethylthiouracil (XXIII), darkens at 260°, m. >360°. XXIII refluxed 6 hrs. in Ac2O gave 3,6,8-trioxopyrimido[5,4-b]-1,4-thiazine, darkens at 300°, m. >360°.

IT 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6,6-dimethoxy-1-propyl-
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-hydroxy-1-propyl-, acetate (ester)
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6,6-diethoxy-3-ethyl-1-propyl-
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-chloro-3-ethyl-1-propyl-

IT 109-12-6, Pyrimidine, 2-amino- (5-alkoxy derivs.)

IT 91184-32-6, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione (derivs.)

IT 1781-12-0, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1,3-dimethyl- 1781-13-1, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6,6-dichloro-3-ethyl-1-propyl- 3950-00-3, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl- 54107-70-9, Uracil, 6-amino-5-chloro- 88513-03-5, Acetic acid, [(6-amino-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)thio]- 90091-31-9, Acetic acid, [(6-amino-1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)thio]- 91184-32-6, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione 91194-51-3, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]- 91338-31-7, Acetic acid, [(1-allyl-6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)thio]- 91978-19-7, Acetic acid, [[6-amino-3-ethyl-1,2,3,4-tetrahydro-1-(2-hydroxyethyl)-2,4-dioxo-5-pyrimidinyl]thio]- 92334-98-0, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-chloro-1,3-dimethyl- 92431-29-3, Acetic acid, [(6-amino-1,3-dibutyl-

1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)thio]- 94216-16-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-(2-hydroxyethyl)- 94216-17-8, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-ethoxy-1,3-dimethyl- 94581-93-8, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-ethoxy-3-ethyl-1-propyl-, 5-oxide 94783-09-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-bromo-3-ethyl-1-propyl- 95046-84-7, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfinyl]-, hydrate 95141-35-8, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-hydroxy-1-propyl- 95141-36-9, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl-, 5-oxide 95141-37-0, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl-, 5,5-dioxide 95709-02-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1-allyl-3-ethyl- 96431-42-4, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,6,7(3H,8H)tetrone, 3-ethyl-1-propyl-, 6-(dimethyl acetal) 96431-43-5, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-ethoxy-3-ethyl-1-propyl- 96434-09-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-methoxy-1-propyl- 96486-26-9, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-(2-chloroethoxy)-3-ethyl-1-propyl- 97319-64-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1,3-dibutyl- 97617-36-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,6,7(3H,8H)tetrone, 3-ethyl-1-propyl-, 6-(diethyl acetal) 97617-37-3, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-butoxy-3-ethyl-1-propyl-
(preparation of)

L38 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1962:442852 HCAPLUS
DN 57:42852
OREF 57:**8574c-i,8575a-i,8576a**
ED Entered STN: 22 Apr 2001
TI The rearrangement of sulfoxides of pyrimido[5,4-b] [1,4]thiazines
AU Schroeder, Elmer F.; Dodson, R. M.
CS G. D. Searle & Co., Chicago
SO Journal of the American Chemical Society (**1962**), 84, 1904-13
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
CC 32 (Heterocyclic Compounds-More than One Hetero Atom)
OS CASREACT 57:42852
AB A series of 1,3-alkylated 5-(carboxymethylthio)-6-aminouracils (I) have been prepared by adding slowly 0.82 mole 80% aqueous thioacetic acid to a stirred suspension of 0.75 mole 1,3-dialkyl-5-chloro-6-aminouracil (II) in 1.65 moles 2.5N NaOH, and heating the mixture at 90° 0.5 hr. Acidification gave I. The following derivs. of I have been prepared: 1,3-dimethyl (III), m. 218-20°, 85%; 1,3-PrEt (IV), m. 182-4°, 90%; 1,3-dibutyl (V), m. 157-9°, 93%; 1-allyl-3ethyl (VI), m. 176-7°, 55%; 1-(β-hydroxyethyl)-3-ethyl, m. 206-7°,42%. A mixture of 45.6 g. IV and 96 ml. Ac2O was heated on a steam bath 4 hrs. and poured into water, cooled, and filtered to give 37.7 g. 1-propyl-3-ethyl-1Hpyrimido [5,4-b] [1,4] thiazine-2,4,7(3H,6H,8H)-trione (VII), m. 186-8° after purification by dissoln. in NaOH and acidification. Similarly the following 1,3-dialkyl-1H-pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione derivs. were obtained: 1,3-Me2, m. 270-2°, 94%; 1,3-Bu2, m. 213-14°, 96%; 1-allyl-3-ethyl, m. 231-3°, 92%; 1-(β-hydroxyethyl)3-ethyl, m. 225-6°, 63%. To a solution of 10.8g. VII in 120 ml. dry alc.-free CHCl3 at 10-15° was added during 0.5 hr. a solution of 5.52 g. BzOOH in 120 ml. dry C6H6. After 1 hr. the mix. was filtered to give 10.8 g. 1-propy-1-3-ethyl-1-H-pyrimido [5,4 b] [1,4] thiazine-2,4,7(3H,6H,8H)-trione 5-oxide (VIII), m. 165-7° (MeCOEt). Addition of 8.1 ml. 40% AcOOH to 14.4 g. IV in a solution of 7 g. NaOH in 150 ml. H2O and stirring 0.5 hr. and acidification gave 12 g. 1 - propyl - 3 - ethyl - 5 - (carboxymethylsulfinyl)-6-aminouracil (IX), m. 100-10° (effervescence). Heating IX in 120 ml. EtOAc gave anhydrous IX, m. 146-7° (decomposition). IX was decomposed by

boiling water to give 1-propyl-3-ethyl-6-aminouracil. Oxidation of 14.4 g. IV in 180 ml. 6% NaOH solution with 18 ml. 40% AcOOH at 10-15° 0.5 hr. gave 12.2 g. 1 - propyl - 3- ethyl - 5 - (carboxymethylsulfonyl)-6-aminouracil (X), m. 205-7° (decomposition). X was more stable than IX. IX could not be cyclized to VIII. A mixture of 9.5 g. X and 19 ml. Ac2O was heated at 100° 4 hrs. Dilution with EtOH gave 6 g. 1-propyl-3-ethyl-1-H-pyrimido [5,4 b] [1,4] thiazine-2,4,7(3H, 6H, 8H)-trione 5,5-dioxide (XI), m. 247-9° (EtOH). XI was strongly acidic and with boiling H2O gave X. In neutral solution XI was quite stable. VIII (19 g.) underwent rearrangement when boiled in EtOH 5 min. to 7.6 g. 1-propyl-3-ethyl-6-ethoxy-1H-pyrimido[5,4-b] [1,4] thiazine-2,4,7(3H,6H,8H)-trione (XII), m. 164-5°. With boiling MeOH VIII gave 1-propyl-3-ethyl-6-methoxy-1H-pyrimido[5,4 b] [1,4] thiazine-2,4,7(3H,6H,8H)-trione (XIII), m. 199-200° (decomposition), λ 323 (ε 8140), 219 mμ (ε 16,200). To a mixture of 13.45 g. VIII and 5 g. NaHCO3 in 120 ml. dry EtOH-free CHCl3 was added 8 g. Br in 50 ml. CHCl3 at 10° and stirred 0.5 hr. Filtration and evaporation gave 17.3 g. 1-propyl-3-ethyl-6-bromo- 1 H- pyrimido [,5,4-b-1][1,4] thiazine-2,4,7(3H,6H,8H)-trione (XIV), m. 197-9° (decomposition),λ 316 mμ (ε 7760). When 17.4 g. XIV was boiled in EtOH 5 min. 14.2 g. XII was obtained. Addition of 8.1 g. SO2Cl2 to 16.2 g. VIII 90 ml. HOAc below 40° gave, after 30 min. at room temperature and addition of 90 ml. hexane at 0°, 16.4 g. 1-propyl-3-ethyl-6-chloro- 1 H-pyrimido [5,4-b] [1,4] thiazine-2,4,7- (3H,6H,8H)-trione (XV), m. 202-5°, λ 315 mμ (ε 8350). Boiled with EtOH 0.5 hr., XV gave XII. When a solution of 2 g. VIII in 8 ml. HOAc was heated 3 min. on a steam bath and diluted with H2O, 1.8 g. 1-propyl-3-ethyl 6-acetoxy-1Hpyrimido[5,4-b] [1,4] thiazine-2,4,7(3H, 6H, 8H)-trione (XVI), m. 159-60° (effervescence) was obtained. XVI was also obtained by heating XIV in HOAc 2 min. When XVI was heated in EtOH 0.5 hr. it gave XII. Spontaneous rearrangement of VIII took place under storage in a dark bottle for 11 months to give 1-propyl-3-ethyl-6-hydroxy-1H-pyrimido[5,4-b][1,4]thiazine (XVII), m. 205-7° (decomposition) (MeCOEt). VIII was also isomerized to XVII by standing in water for 24 hrs. Heating XVI with water 15 min. also gave XVII. When 1 g. XVII was heated with 15 ml. absolute EtOH and 3 drops concentrated H2SO4 1 hr. and the solo. diluted, 0.54 g. XII was obtained. To a stirred solution of 15.7 g. XII in 60 ml. HOAc was added slowly 10 ml. of 40%. AcOOH in HOAc at 30-40° and the mixture kept at room temperature 0.5 hr. and diluted with 200 ml. H2O gave 10.3 g. 1-propyl-3-ethyl-6-ethoxy-1H-pyrmido [5,4 - b] [1,4] thiazine - 2,4,7(3H,6H,8H)- tri one 5-oxide (XVIII), m. 186-7°. A suspension of 10 g. XVIII in 100 ml. absolute EtOH was refluxed 4 hrs. Concentration and dilution gave 6.4 g. 1-propyl-3-ethyl-6,6-diethoxy-] H-pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione (XIX) m. 165-7° (EtOH). A solution of 26.9 g. IV in 250 ml. dry CCl4 was refluxed with 27 g. SO2Cl2 1.5 hrs. and heated with 50 ml. hexane to give 20.5 g. 1-propyl-3-ethyl-6,6-dichloro-1H-pyrimido[5,4-b] [1,4]thiazine-2,4,7(3H,6H,8H)-trione (XX), m. 145-7° (decomposition) λ 316 mμ (ε 6900). When a solution of 2 g. IV was kept in 6 ml. concentrated NH4OH at room temperature 6 days 2.08 g. 1-propyl-3-ethyl-5-(carbamoylmethylthio)-6-aminouracil (XXI), m. 204-6° (EtOH) was obtained. Similar reactions with MeNH2 and PrNH2 gave 1 propyl-3-ethyl - 5 - (N- methylcarbamoylmethylthio - 6 - aminouracil (XXII), m. 185-7° and the corresponding N-Pr derivative, m. 102-3°; anhyd, m. 158-9°. Treatment of XI with concentrated NH4OH gave in 74% yield 1-propyl-3-ethyl-5-(carbamoylmethanesulfonyl)-6-aminouracil (XXIII), m. 236-8°. When XXIII was heated with NaOH, IV was obtained. XI and Me-NH2 gave the N-methyl derivative of XXIII, m. 197-9°. A solution of 4.4 g. XII in 15 ml. concentrated NH4OH was allowed to stand at room temperature 3 days to give 3.55 g. 1-propyl-3-ethyl-5-(carbamoylethoxymethylthio)-6-aminouracil (XXIV), m. 222-3° (decomposition), besides some recovered XII. Use of MeNH2 gave 1-propyl-3-ethyl-5-(N-methylcarbamoyleth-oxymethylthio)-6-aminouracil (XXV), m. 164-6°, 98% yield. Treatment of XIX with concentrated NH4OH 13 days at room temperature gave 1-propyl-3-ethyl-5-(carbamoyldiethoxy-methylthio)-

6-aminouracil (XXVI), m. 188-9°. When XXVI was heated in water 2 hrs. it gave a bright yellow compound, m. 257-8°. The structures of XII and XXIV were proven by desulfurization of 3.00 g. XXVI with Raney Ni in refluxing EtOH for 3 hrs. EtOH was evaporated and H2O added to give 1.6 g. 1-propyl 3-ethyl-6-aminouracil (XXVII), m. 170-2°. The aqueous filtrate from XXVII was evaporated to dryness to give 0.2 g. ethoxyacetamide (XXVIII), m. 79-81°. XVIII (10 g.) mixed with 30 ml. concentrated XH4OH and left overnight gave 7.6 g. 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propylthiazolo [4,5-d] pyrimidine-2-carboxamide (XXIX), m. 186-8°,λ225(ε20,300),337 mμ (ε6150). A mixture of 10g. XX and 30 ml. HOAc was heated 20 min. on a steam bath. On cooling 1-propyl-3-ethyl-1H-pyrimido[5,4-b] [1,4]thiazine-2,4,6,7(3H,8H)-tetraone (XXX), m. 237-8°, X 227 (ε 19,400), 340 mμ (ε 6060) was obtained. When XXX was treated with concentrated NH4OH at room temperature 2.5 hrs. XXIX was obtained in 85% yield. Similarly with MeNH2 XXX gave 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propylthiazolo[4,5-d]pyrimidine-2-N-methylcarboxamide (XXXI), m. 1801°. Me2NH gave the corresponding N,N-dimethylcarboxamide (XXXII), m. 111-12° in 52% yield. 2 Amino-ethanol gave the corresponding N-(β-hydroxyethyl)carboxamide (XXXIII), m. 125-7°. A suspension of 2.4 g. XXX in 20 ml. absolute EtOH was refluxed 1 hr., cooled, and diluted to give 2.1 g. ethyl 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4propylthiazolo[4,5-d]pyrimidine-2-carboxylate (XXXIV), m. 81-2°. The amides XXIX, XXXI, XXXII, and XXXIII could also be obtained from XXXIV. XXXIV (0.94 g.) was hydrolyzed with 10 ml. 0.5N NaOH at room temperature 0.5 hr. Acidification gave 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propylthiazolo [4,5-d] pyrimidine-2-carboxylic acid (XXXV), m. 102-4° (decomposition) (monohydrate), 130-2° (decomposition) (anhydrous). XXXV could also be obtained from XXX in 83% yield by treatment with N NaOH solo. at room temperature 0.5 hr. XXXV (4.5 g.) heated at 135-40° 0.5 hr. gave 3.7 g. 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4propylthiazolo[4,5-d]pyrimidine, m. 78-9° (aqueous EtOH).

IT Rearrangements
(of 1H-pyrimido[5,4-b][1,4]thiazine 5-oxide derivs.)

IT 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6,6-dimethoxy-1-propyl-
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-hydroxy-1-propyl-, acetate (ester)
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6,6-diethoxy-3-ethyl-1-propyl-
1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-chloro-3-ethyl-1-propyl-
2,3-Dlazabicyclo[2.2.2]oct-2-ene
Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfonyl]-N-methyl-
Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-2-ethoxy-
Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-2-ethoxy-N-methyl-
Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-N-methyl-
Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-N-propyl-, hydrate

IT 1H-Pyrimido[5,4-b][1,4]thiazine, 5-oxide
(derivs., rearrangements of)

IT 7727-37-9, Nitrogen
(compds., heterocyclic)

IT 884-75-3, Phosphinic amide, P,P-bis(1-aziridinyl)-N-(5-chloro-2-pyrimidinyl)- 1781-10-8, Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- 1781-11-9, Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-methyl-5,7-dioxo-4-propyl- 1781-12-0, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1,3-dimethyl- 1781-13-1, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6,6-dichloro-3-ethyl-1-propyl- 1781-20-0, Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- 1781-21-1,

Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl-, ethyl ester 2937-31-7, Phosphinic amide, P,P-bis(1-aziridinyl)-N-(4-methyl-2-pyrimidinyl)- 2937-35-1, Phosphinic amide, P,P-bis(1-aziridinyl)-N-[4-(diethylamino)-2-pyrimidinyl]- 3408-51-3, Phosphinic amide, P,P-bis(1-aziridinyl)-N-(4,6-dimethyl-2-pyrimidinyl)- 3758-26-7, Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 6-ethyl-4-propyl- 3758-28-9, Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N,N-dimethyl-5,7-dioxo-4-propyl- 3764-09-8, Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-(2-hydroxy-ethyl)-5,7-dioxo-4-propyl- 3764-10-1, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,6,7(3H,8H)tetrone, 3-ethyl-1-propyl- 3880-49-7, Azoethane, 1,1'-dimethyl- 3950-00-3, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl- 51770-98-0, Acetamide, 2-ethoxy- 63981-32-8, Uracil, 6-amino-3-ethyl-1-propyl- 90091-31-9, Acetic acid, [(6-amino-1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)thio]- 90485-45-3, Pyridazine, 3,4,5,6-tetrahydro-3,6-dimethyl- 91194-51-3, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]- 91253-34-8, Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]- 91253-39-3, Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfonyl]- 91338-31-7, Acetic acid, [(1-allyl-6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)thio]- 91978-19-7, Acetic acid, [[6-amino-3-ethyl-1,2,3,4-tetrahydro-1-(2-hydroxyethyl)-2,4-dioxo-5-pyrimidinyl]thio]- 92107-80-7, Glyoxylamide, S-(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl) O-Et monothioacetal 92370-43-9, Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-N-propyl- 92370-45-1, Glyoxylamide, N-methyl-, S-(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl) O-Et monothioacetal 92431-29-3, Acetic acid, [(6-amino-1,3-dibutyl-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)thio]- 92575-67-2, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfonyl]- 94216-16-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-(2-hydroxyethyl)- 94581-93-8, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-ethoxy-3-ethyl-1-propyl-, 5-oxide 94783-09-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-bromo-3-ethyl-1-propyl- 95046-83-6, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfinyl]- 95046-84-7, Acetic acid, [(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)sulfinyl]-, hydrate 95141-35-8, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-hydroxy-1-propyl- 95141-36-9, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl-, 5-oxide 95141-37-0, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-1-propyl-, 5,5-dioxide 95389-27-8, Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl-, hydrate 95709-02-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1-allyl-3-ethyl- 96431-42-4, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,6,7(3H,8H)tetrone, 3-ethyl-1-propyl-, 6-(dimethyl acetal) 96431-43-5, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 6-ethoxy-3-ethyl-1-propyl- 96434-09-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-methoxy-1-propyl- 97319-64-7, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 1,3-dibutyl- 97525-58-1, Acetamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-2,2-diethoxy- 97525-58-1, Glyoxylamide, 2-[(6-amino-3-ethyl-1,2,3,4-tetrahydro-2,4-dioxo-1-propyl-5-pyrimidinyl)thio]-, 2-(diethyl acetal) 97617-36-2, 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,6,7(3H,8H)tetrone, 3-ethyl-1-propyl-, 6-(diethyl acetal)
(preparation of)

L38 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1962:442851 HCAPLUS
DN 57:42851
OREF 57:8573h-i,8574a-c

Search done by Noble Jarrell

ED Entered STN: 22 Apr 2001
TI Ethylenimine derivatives. III. Diethylenamides of pyrimidylphosphoramidic acids
AU Kropacheva, A. A.; Sazonov, N. V.
CS S. Ordzhonikidze All-Union Chem.-Pharm. Res. Inst., Moscow
SO Zhurnal Obshchei Khimii (1961), 31, 3601-5
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Unavailable
CC 32 (Heterocyclic Compounds-More than One Hetero Atom)
AB cf. CA 55, 18695a. Adding 4 g. 2-amino-4-methoxypyrimidine to 10 ml. POCl3 in C6H6 and heating 5 hrs. at 45-50° gave a precipitate of the pyrimidine-HCl and N-(4.methoxy-2pyrimidyl)phosphoramidic dichloride (I); this heated with 2:1 C6H6-CHCl3 left the residue of the former, while filtration, and evaporation of the filtrate gave 62% I, m. 190°. Similarly were prepared 4-diethylamino-2-pyrimidyl and 4,6-dimethyl-2-pyrimidyl analogs which could not be purified satisfactorily. 2-Amino-4-chloropyrimidine and 5-chloro-2-aminopyrimidine required refluxing with excess POCl3 for unstated periods for complete reaction and gave the N-derivs. of phosphoramidic dichlorides: 4-chloro-2-pyrimidyl, m. 163-4°, 84.3%; and 5-chloro-2-pyrimidyl, m. 163-3.5°. Refluxing 2-amino-4-methylpyrimidine-HCl with excess POCl3 until dissolved gave after evaporation in vacuo 56.5% N-(4-methyl-2-pyrimidyl)phosphoramidic dichloride, m. 164-5°; similarly was prepared 73.5% the 4-benzylmethyl-2pyrimidyl analog, m. 190°, and 2-pyrimidyl analog, m. 171-2°. Addition of the dichlorides to ethylenimine in C6H6 in the presence of Et3N with cooling, followed by stirring 2 hrs. at room temperature and standing overnight gave after brief heating and filtration while hot from the amine-HCl precipitate, followed by evaporation, the following RNHP(O)[N(CH2)2]2 (R shown): 2-pyrimidyl, m. 128-9°, 78%; 4-chloro-2-pyrimidyl, decomposed at 121 2°, 45%; 4 (N-aziridyl)-2-pyrimidyl, decomposed at 129-30°, 21.6%; 4-methoxy-2-pyrimidyl, m. 128-9°, 77%; 4-benzylmethylamino-2-pyrimidyl, m. 151-2.5°, 48%; 4-methyl-2-pyrimidyl, m. 1234°, 75.8%; 5-chloro-2-pyrimidyl, decomposed at 157-8°, 83.4%; 4-diethylamino-2-pyrimidyl, m. 150-50.5°, 53.8%; 4,6-dimethyl-2-pyrimidyl; m. 128-9°, 80.8%. These ethylenimine derivs. were prepared for biol. tests.
IT 151-56-4, Ethylenimine 882-58-6, Phosphinic amide, P,P-bis(1-aziridinyl)-N-pyrimidinyl-
(derivs.)
IT 780-66-5, Phosphinic amide, P,P-bis(1-aziridinyl)-N-(4-chloro-2-pyrimidinyl)- 882-58-6, Phosphinic amide, P,P-bis(1-aziridinyl)-N-2-pyrimidinyl- 2937-32-8, Phosphinic amide, P,P-bis(1-aziridinyl)-N-(4-methoxy-2-pyrimidinyl)- 2937-34-0, Phosphinic amide, P,P-bis(1-aziridinyl)-N-[4-(1-aziridinyl)-2-pyrimidinyl]- 2937-35-1, Phosphinic amide, P,P-bis(1-aziridinyl)-N-[4-(diethylamino)-2-pyrimidinyl]- 2937-36-2, Phosphinic amide, P,P-bis(1-aziridinyl)-N-[4-(benzylmethylamino)-2-pyrimidinyl]- 4270-12-6, Phosphoramidic dichloride, (5-chloro-2-pyrimidinyl)- 4270-13-7, Phosphoramidic dichloride, (4-chloro-2-pyrimidinyl)- 4270-19-3, Phosphoramidic dichloride, 2-pyrimidinyl- 4270-20-6, Phosphoramidic dichloride, (4-methyl-2-pyrimidinyl)- 4270-21-7, Phosphoramidic dichloride, (4-methoxy-2-pyrimidinyl)- 91761-23-8, 2H-1,2-Thiazine, tetrahydro-2-(3-pyridylmethyl)-, 1,1-dioxide 95196-88-6, Phosphoramidic dichloride, [4-(benzylmethylamino)-2-pyrimidinyl]-
(preparation of)

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L35 ANSWER 1 OF 5 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA63:7781h CAOLD
TI electron spectroscopic determination of the directions of transition and of the ionization and tautomerism consts. of 7-hydroxylumazine and of its methyl derivs.
AU Prigge, Helmut; Lippert, E.
IT 2577-38-0 2614-42-8 2614-43-9 2614-44-0 2622-65-3 2622-66-4
2625-21-0 2625-22-1 2625-23-2 2744-64-1 3215-22-3
3215-23-4 3220-42-6 3220-43-7 3221-08-7 31053-46-0
90971-99-6

L35 ANSWER 2 OF 5 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA61:7025b CAOLD
TI pyrazolo[3,4-d]pyrimidines
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DT Patent

PATENT NO.	KIND	DATE
GB 937725		

IT 92165-44-1 92871-93-7 93117-35-2 93738-68-2 93738-69-3
94030-23-6 94548-52-4 94916-12-8 94994-79-3 96267-34-4 96368-88-6
96732-25-1 97864-53-4 98132-44-6

L35 ANSWER 3 OF 5 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA61:7024h CAOLD
TI pyrido[2,3-d]pyrimidine-2,4,5,7-tetraones
AU Scarborough, Homer C.
PA Mead Johnson & Co.
DT Patent

PATENT NO.	KIND	DATE
US 3139432		1964
GB 989048		

IT 91996-75-7 93117-36-3 93738-66-0 93738-67-1 95709-04-9
96986-13-9 97360-49-1

L35 ANSWER 4 OF 5 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA59:6420h CAOLD
TI 3,6,8-trioxopyrimido(5,4-b)-1,4-thiazines
PA Searle, G. D., & Co.
DT Patent
TI 3,6,8-trioxopyrimido[5,4-b][1,4]thiazines
AU Schroeder, Elmer F.
DT Patent

PATENT NO.	KIND	DATE
US 3080364		1963

IT 1781-12-0 1781-13-1 3950-00-3 54107-70-9 88513-03-5 90091-31-9

91194-51-3 91338-31-7 91978-19-7 92334-98-0 92431-29-3 94216-16-7
94216-17-8 94581-93-8 94783-09-2 95141-35-8 95141-36-9 95141-37-0
95709-02-7 96431-42-4 96431-43-5 96434-09-2 96486-26-9
96732-27-3 97319-64-7 97617-36-2 97617-37-3

L35 ANSWER 5 OF 5 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA57:8574c CAOLD
TI rearrangement of sulfoxides of pyrimido [5,4-b][1,4]thiazines
AU Schroeder, Elmer F.; Dodson, R. M.
IT 884-75-3 1781-10-8 1781-12-0 1781-13-1 1781-20-0 1781-21-1
2937-31-7 2937-35-1 3408-51-3 3758-28-9 3764-09-8 3764-10-1
3950-00-3 51770-98-0 63981-32-8 90091-31-9 91194-51-3 91253-34-8
91253-39-3 91338-31-7 91978-19-7 92107-80-7 92370-43-9 92370-45-1
92431-29-3 92575-67-2 94216-16-7 94581-93-8 94783-09-2 95046-83-6
95046-84-7 95141-35-8 95141-36-9 95141-37-0 95389-27-8 95709-02-7
96431-42-4 96431-43-5 96434-09-2 96732-27-3 97319-64-7
97525-58-1 97617-36-2

=> b reg
FILE 'REGISTRY' ENTERED AT 08:45:17 ON 07 JUL 2005
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STRUCTURE FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9
DICTIONARY FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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conducting SmartSELECT searches.

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*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005. A new display format, IDERL, is now      *
* available and contains the CA role and document type information.  *
*                                                                    *
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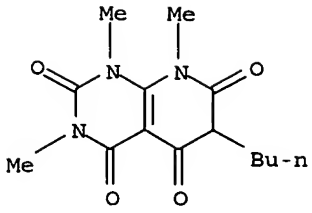
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l39 tot

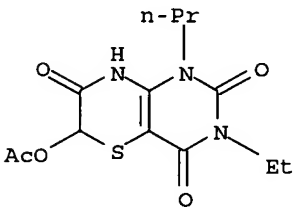
L39 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN 97864-53-4 REGISTRY
ED Entered STN: 31 Aug 1985
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3,8-
trimethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H19 N3 O4
SR CAOLD
LC STN Files: CA, CAOLD, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

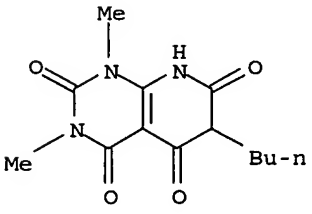
L39 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN 96732-27-3 REGISTRY
ED Entered STN: 15 Jun 1985
CN 1H-Pyrimido[5,4-b][1,4]thiazine-2,4,7(3H,6H,8H)-trione, 3-ethyl-6-hydroxy-1-propyl-, acetate (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 N3 O5 S
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L39 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN 96732-25-1 REGISTRY
ED Entered STN: 15 Jun 1985
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3-dimethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 N3 O4
LC STN Files: CA, CAOLD, CAPLUS



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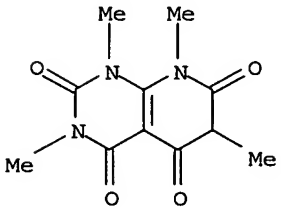
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L39 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN **95709-04-9** REGISTRY
ED Entered STN: 06 Apr 1985
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6,8-tetramethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H13 N3 O4
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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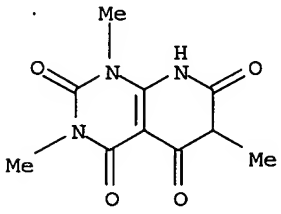
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L39 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN **93738-69-3** REGISTRY
ED Entered STN: 18 Dec 1984
CN Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6-trimethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H11 N3 O4
LC STN Files: CA, CAOLD, CAPLUS



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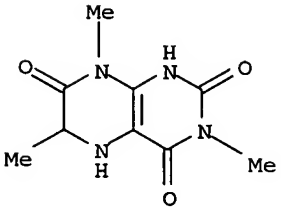
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L39 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN **3215-23-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-3,6,8-trimethyl- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD

MF C9 H12 N4 O3
LC STN Files: CA, CAOLD, CAPLUS



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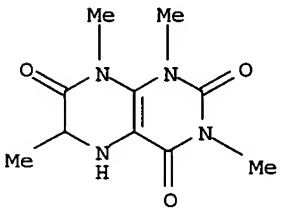
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L39 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN
RN 3215-22-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,4,7(1H,3H,6H)-Pteridinetrione, 5,8-dihydro-1,3,6,8-tetramethyl- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H14 N4 O3
LC STN Files: CA, CAOLD, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> b home
FILE 'HOME' ENTERED AT 08:45:29 ON 07 JUL 2005

=>

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=> d his full 20

     FILE 'REGISTRY' ENTERED AT 09:03:25 ON 07 JUL 2005
L41             STR L5
L42          12 SEA SSS SAM L41 AND L1 AND (L2 OR L3) AND L4
L43         299 SEA SSS FUL L41 AND L1 AND (L2 OR L3) AND L4
                SAV TEM WAR489F1/A L43
                D QUE L9
L44             STR L9
L45             STR L12
L46             STR L15
L47           0 SEA SUB=L43 SSS SAM L44
L48          26 SEA SUB=L43 SSS FUL L44
L49           2 SEA SUB=L43 SSS SAM L45
L50          21 SEA SUB=L43 SSS FUL L45
L51           4 SEA SUB=L43 SSS SAM L46
L52         103 SEA SUB=L43 SSS FUL L46
                SAV TEM L48 WAR489S3/A
                SAV TEM L50 WAR489S4/A
                SAV TEM L52 WAR489S5/A

     FILE 'HCAPLUS' ENTERED AT 09:09:22 ON 07 JUL 2005
L53          30 SEA ABB=ON  PLU=ON  L48 OR L50 OR L52

     FILE 'HCAOLD' ENTERED AT 09:09:39 ON 07 JUL 2005
L54           6 SEA ABB=ON  PLU=ON  L48 OR L50 OR L52
                SEL AN
                EDIT E13-E18 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 09:10:00 ON 07 JUL 2005
L55          10 SEA ABB=ON  PLU=ON  ("CA52:18457H"/OREF OR "CA53:1364F"/OREF
                OR "CA57:8569G"/OREF OR "CA60:8027F"/OREF OR "CA61:7024H"/OREF
                OR "CA65:2260C"/OREF)
L56           1 SEA ABB=ON  PLU=ON  (L53 OR L55) AND (L18 OR L19)
L57          33 SEA ABB=ON  PLU=ON  (L53 OR L55) NOT L56
L58          32 SEA ABB=ON  PLU=ON  L57 AND L32
L59          33 SEA ABB=ON  PLU=ON  (L57 OR L58)

     FILE 'HCAOLD' ENTERED AT 09:11:44 ON 07 JUL 2005
                SEL HIT RN L54

     FILE 'REGISTRY' ENTERED AT 09:11:59 ON 07 JUL 2005
L60           9 SEA ABB=ON  PLU=ON  (6743-26-6/RN OR 91769-67-4/RN OR 97360-49-
                1/RN OR 90324-12-2/RN OR 93318-04-8/RN OR 95296-09-6/RN OR
                95709-05-0/RN OR 99069-70-2/RN OR 99073-13-9/RN)

=> b reg
FILE 'REGISTRY' ENTERED AT 09:13:31 ON 07 JUL 2005
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STRUCTURE FILE UPDATES:    6 JUL 2005  HIGHEST RN 853990-77-9
DICTIONARY FILE UPDATES:   6 JUL 2005  HIGHEST RN 853990-77-9

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************

                        Search done by Noble Jarrell
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*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d que sta l48
L1              SCR 1839 AND 1994 AND 2005 AND 1440
L2              SCR 1264
L3              SCR 1210 AND 1263
L4              SCR 1029 OR 1107 OR 1141 OR 1156
L41             STR
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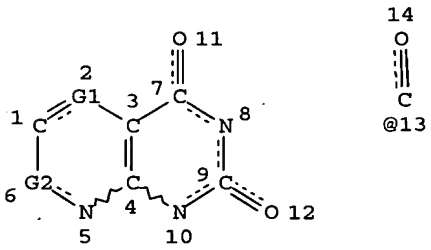


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VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L43          299 SEA FILE=REGISTRY SSS FUL L41 AND L1 AND (L2 OR L3) AND L4
L44             STR
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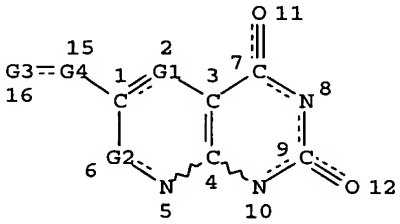

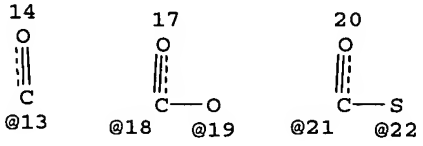

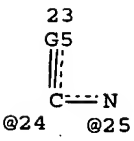


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VAR G1=C/O/S/N
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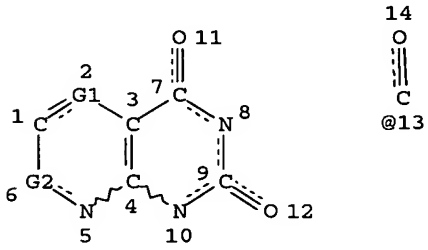
VAR G2=CH2/13
VAR G3=AK/CY
VAR G4=CY/18-1 19-16/18-16 19-1/21-1 22-16/21-16 22-1/24-1 25-16/25-1 24-16
VAR G5=O/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L48 26 SEA FILE=REGISTRY SUB=L43 SSS FUL L44

100.0% PROCESSED 299 ITERATIONS 26 ANSWERS
SEARCH TIME: 00.00.01

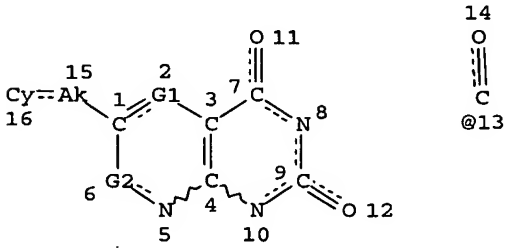
=> d que sta l50
L1 SCR 1839 AND 1994 AND 2005 AND 1440
L2 SCR 1264
L3 SCR 1210 AND 1263
L4 SCR 1029 OR 1107 OR 1141 OR 1156
L41 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L43 299 SEA FILE=REGISTRY SSS FUL L41 AND L1 AND (L2 OR L3) AND L4
L45 STR



VAR G1=C/O/S/N
VAR G2=CH2/13

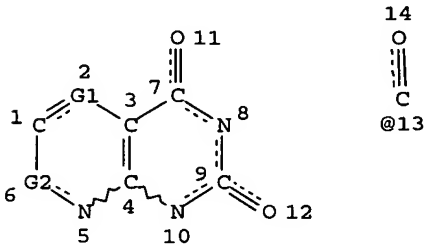
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L50 21 SEA FILE=REGISTRY SUB=L43 SSS FUL L45

100.0% PROCESSED 299 ITERATIONS 21 ANSWERS
SEARCH TIME: 00.00.01

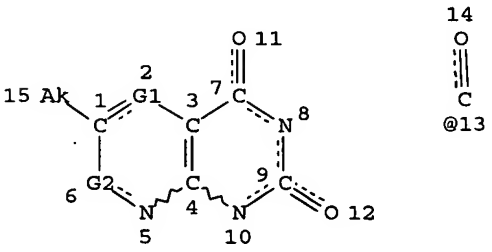
=> d que sta l52
L1 SCR 1839 AND 1994 AND 2005 AND 1440
L2 SCR 1264
L3 SCR 1210 AND 1263
L4 SCR 1029 OR 1107 OR 1141 OR 1156
L41 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L43 299 SEA FILE=REGISTRY SSS FUL L41 AND L1 AND (L2 OR L3) AND L4
L46 STR



VAR G1=C/O/S/N
VAR G2=CH2/13
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L52         103 SEA FILE=REGISTRY SUB=L43 SSS FUL L46

100.0% PROCESSED     299 ITERATIONS                          103 ANSWERS
SEARCH TIME: 00.00.01


=> b hcap
FILE 'HCAPLUS' ENTERED AT 09:13:51 ON 07 JUL 2005
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FILE COVERS 1907 - 7 Jul 2005  VOL 143 ISS 2
FILE LAST UPDATED: 6 Jul 2005  (20050706/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d all fhitstr l56

L56  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:143163  HCAPLUS
DN   140:175195
ED   Entered STN:  22 Feb 2004
TI   5,6-Fused uracil derivatives as matrix metalloproteinase inhibitors,
     pharmaceutical compositions, and therapeutic use
IN   Roark, William Howard
PA   Warner-Lambert Company LLC, USA
SO   PCT Int. Appl., 193 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  C07D495-04
     ICS  C07D471-04; A61K031-519; A61P019-02
CC   1-12 (Pharmacology)
     Section cross-reference(s): 63
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
PI   WO 2004014921         A1    20040219    WO 2003-IB3505          20030804
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
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FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004224951 A1 20041111 US 2003-634489 20030805
PRAI US 2002-403037P P 20020813
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004014921	ICM	C07D495-04
	ICS	C07D471-04; A61K031-519; A61P019-02
WO 2004014921	ECLA	C07D471/04+239B+221B; C07D495/04+335B+239B
US 2004224951	NCL	514/242.000; 514/262.100; 514/264.100; 544/184.000; 544/256.000; 544/279.000
	ECLA	C07D471/04+239B+221B; C07D495/04+335B+239B

OS MARPAT 140:175195

AB The invention provides 5,6-fused uracil derivs.,or pharmaceutically acceptable salts thereof. The invention also provides pharmaceutical compns. comprising a compound of the invention, or a pharmaceutically acceptable salt thereof, together with a pharmaceutically acceptable carrier, diluent, or excipient. The invention also provides methods of inhibiting a MMP-13 enzyme in an animal, comprising administering a compound of the invention, or a pharmaceutically acceptable salt thereof. The invention also provides methods of treating a disease mediated by an MMP-13 enzyme in a patient, comprising administering to the patient a compound of the invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition The invention also provides methods of treating diseases such as heart disease, multiple sclerosis, osteo- and rheumatoid arthritis, arthritis other than osteo- or rheumatoid arthritis, cardiac insufficiency, inflammatory bowel disease, heart failure, age-related macular degeneration, chronic obstructive pulmonary disease, asthma, periodontal diseases, psoriasis, atherosclerosis, and osteoporosis in a patient, comprising administering to the patient a compound of the invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition The invention also provides combinations, comprising a compound of the invention, or a pharmaceutically acceptable salt thereof, together with another pharmaceutically active component.

ST fused uracil deriv matrix metalloproteinase inhibitor therapeutic

IT Drug delivery systems
(capsules; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Ampuls
Antiarthritics
Arthritis
Drug delivery systems
Human
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(injections; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(ointments; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(solns.; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(suppositories; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(tablets, coated; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT Drug delivery systems
(tablets; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT 141907-41-7, Matrix metalloproteinase

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

IT 657350-98-6 657350-99-7 657351-00-3 657351-01-4 657351-02-5
657351-03-6 **657351-04-7** 657351-05-8
657351-06-9 657351-07-0 657351-08-1
657351-09-2 657351-10-5 657351-11-6
657351-12-7 657351-13-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

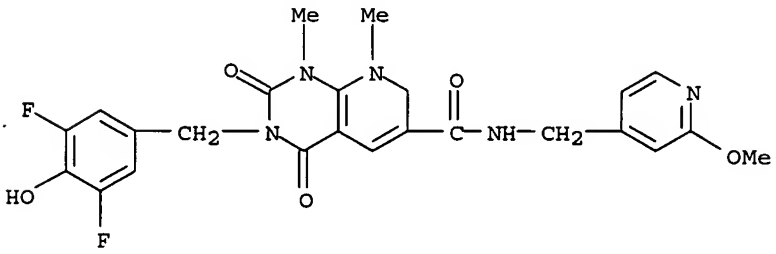
IT 169590-42-5, Celecoxib 181695-72-7, Valdecoxib
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., therapeutic use, and use with other agents)

IT 329900-75-6, Cyclooxygenase 2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., therapeutic use, and use with other agents)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Ibfb Gmbh; DE 10101324 C 2001 HCAPLUS
(2) Ibfb Gmbh; DE 19940494 C 2001 HCAPLUS
(3) Warner-Lambert Company; WO 02064572 A 2002 HCAPLUS
(4) Warner-Lambert Company; WO 02064598 A 2002 HCAPLUS
(5) Warner-Lambert Company; WO 03033477 A 2003 HCAPLUS
(6) Warner-Lambert Company; WO 03033478 A 2003 HCAPLUS

IT **657351-04-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fused uracil derivs. as matrix metalloproteinase inhibitors, pharmaceutical compns., and therapeutic use)

RN 657351-04-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxamide, 3-[(3,5-difluoro-4-hydroxyphenyl)methyl]-1,2,3,4,7,8-hexahydro-N-[(2-methoxy-4-pyridinyl)methyl]-1,8-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



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L59 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:927010 HCAPLUS
DN 141:376382
ED Entered STN: 04 Nov 2004
TI Pin1-modulating compounds and methods of use for the treatment of Pin1-associated diseases, including cancer
IN Bao, Lere; Kimzey, Amy
PA Pintex Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 189 pp.

CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 1, 27, 28
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004093803	A2	20041104	WO 2004-US11957	20040416

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO; SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-463271P P 20030416
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004093803	ICM	A61K

OS MARPAT 141:376382
AB The invention is directed to modulators, e.g., inhibitors, of Pin1 and Pin1-related proteins and the use of such modulators for treatment of Pin1 associated states, e.g., for the treatment of cancer. The present invention aims to provide photochemotherapeutic compds. with increased specificity as compared with known agents.
ST Pin1 modulator therapeutic cancer treatment
IT Cyclins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(D1; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Skin
(Merkel cell, cancer; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adrenal gland, neoplasm
Antitumor agents
Drug delivery systems
Esophagus, neoplasm
Hodgkin's disease
Human
Lymphoma
Mammary gland, neoplasm
Melanoma
Mouth, neoplasm
Neoplasm
Ovary, neoplasm
Pheochromocytoma
Prostate gland, neoplasm
Sarcoma
Testis, neoplasm
Transformation, neoplastic
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Transforming proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Aldehydes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Pin1-modulating compds. for treatment of Pin1-associated diseases,

including cancer)
IT Apoptosis
Photodynamic therapy
Photosensitizers, pharmaceutical
Radiotherapy
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Interleukin 2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Interleukin 2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Esophagus, neoplasm
Gallbladder, neoplasm
Lung, neoplasm
Pancreas, neoplasm
Parathyroid gland, neoplasm
Stomach, neoplasm
(adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adrenal gland, neoplasm
(adenoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adenoma
(adrenal; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm
(astrocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Skin, neoplasm
(basolioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(bladder transitional cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Sarcoma
(carcinosarcoma, uterus; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(carcinosarcoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(cervix, carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(cervix; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(colon adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon, adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon, adenoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adenoma
(colonic; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Carcinoma
(cutaneous squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT DNA
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(damage; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(endometrial; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(endometrioid; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(endometrium, carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(esophageal adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(follicular and adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(gastric adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm
(glioblastoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(hepatocellular; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Liver, neoplasm
(hepatoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Hyperplasia
(inhibitors; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Lung, neoplasm
(large cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adipose tissue, neoplasm
(lipoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adipose tissue, neoplasm
Sarcoma
(liposarcoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(medullary carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lymphoma
(mucosa-associated lymphoid tissue; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Astrocyte
(neoplasm, astrocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Oligodendrocyte
(neoplasm, oligodendroglioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Skin, disease
(nevus; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lymphoma
(non-Hodgkin's; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm

(oligodendroglioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Kidney, neoplasm
(oncocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(oncogenic; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Ras proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(p21c-Ha-ras; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Ras proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(p21c-Ha-ras; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Carcinoma
(pancreatic adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(papillary carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary small-cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Kidney, neoplasm
(renal cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(renal cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Testis, neoplasm
(seminoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(small, adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lung, neoplasm
(small-cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lung, neoplasm
Skin, neoplasm
Skin, neoplasm
(squamous cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thymus gland, neoplasm
(thymoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(thyroid medullary; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(thyroid papillary; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Bladder, neoplasm
(transitional cell carcinoma; Pin1-modulating compds. for treatment of

Pin1-associated diseases, including cancer)

IT 415965-81-0, Prolyl isomerase Pin1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 536-17-4 3785-78-2 4649-06-3 4703-96-2 6594-02-1 7025-19-6
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

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676644-30-7 676644-32-9 676644-36-3 676644-38-5 676644-40-9
676644-41-0 676644-43-2 676644-49-8 676644-50-1 676644-52-3
676644-56-7 676644-58-9 676644-63-6 676644-69-2 676644-71-6
676644-75-0 676644-79-4 676644-83-0 676644-85-2 676644-86-3
676644-88-5 676644-91-0 676644-95-4 676644-99-8 676645-01-5
676645-03-7 676645-06-0 676645-09-3 676645-13-9 676645-18-4
676645-20-8 676645-21-9 676645-23-1 676645-24-2 676645-40-2
676645-50-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676645-55-9 676645-56-0 676645-58-2 676645-60-6 676645-62-8
676645-64-0 676645-66-2 676645-67-3 676645-69-5 676645-70-8
676645-71-9 676645-74-2 676645-79-7 676645-81-1 676645-82-2
676645-83-3 676645-85-5 676645-86-6 676645-90-2 676645-92-4
676645-94-6 676646-07-4 676646-20-1 676646-26-7 676646-27-8
676646-28-9 676646-30-3 676646-32-5 676646-34-7 676646-37-0
676646-39-2 676646-41-6 676646-42-7 676646-44-9 676646-46-1
676646-48-3 676646-50-7 676646-52-9 676646-53-0 676646-54-1
676646-56-3 676646-58-5 676646-60-9 676646-61-0 676646-62-1
676646-63-2 676646-64-3 676646-65-4 676646-70-1 676646-72-3
676646-74-5 676646-76-7 676646-78-9 676646-80-3 676646-81-4
676646-83-6 676646-85-8 676646-86-9 676646-88-1 676646-90-5
676646-92-7 676646-94-9 676646-95-0 676646-96-1 676646-97-2
676646-98-3 676646-99-4 676647-00-0 676647-01-1 676647-02-2
676647-03-3 676647-04-4 676647-05-5 676647-06-6 676647-07-7
676647-08-8 676647-09-9 676647-10-2 676647-11-3 676647-12-4
676647-13-5 676647-14-6 676647-15-7 676647-16-8 676647-17-9
676647-18-0 676647-19-1 676647-20-4 676647-21-5 676647-22-6
676647-23-7 676647-24-8 676647-25-9 676647-26-0 676647-28-2
676647-29-3 676647-31-7 676647-32-8 676647-33-9 676647-34-0
676647-61-3 676647-62-4 676647-63-5 676647-64-6 676647-65-7
676647-66-8 676647-67-9 676647-68-0 676647-69-1 676647-70-4
676647-71-5 676647-72-6 676647-73-7 676647-74-8 676647-75-9
676647-76-0 676647-77-1 676647-78-2 676647-79-3 676647-80-6

676647-81-7 676647-82-8 676647-84-0 676647-86-2 676647-87-3
676647-88-4 676647-89-5 676647-90-8 676647-91-9 676647-92-0
676647-93-1 676647-94-2 676647-95-3 676647-96-4 676647-97-5
676647-98-6 676647-99-7 676648-00-3 676648-01-4 676648-02-5
676648-03-6 676648-04-7 676648-05-8 676648-06-9 676648-07-0
676648-08-1 676648-09-2 676648-10-5 676648-11-6 676648-12-7
676648-13-8 676648-14-9 676648-15-0 676648-16-1 676648-17-2
676648-18-3 676648-19-4 676648-20-7 676648-21-8 676648-22-9
676648-23-0 676648-24-1 676648-25-2 676648-26-3 676648-27-4
676648-28-5 676648-29-6 676648-30-9 676648-31-0 676648-32-1
676648-33-2 676648-34-3 676648-35-4 676648-36-5 676648-37-6
676648-38-7 676648-39-8 676648-40-1 676648-41-2 676648-42-3
676648-43-4 676648-44-5 676648-45-6 676648-46-7 676648-47-8
676648-48-9 676648-49-0 676648-50-3 676648-51-4 676648-52-5
676648-53-6 676648-54-7 676648-55-8 676648-56-9 676648-57-0
676648-58-1 676648-59-2 676648-60-5 676648-61-6 676648-62-7
676648-63-8 676648-64-9 676648-65-0 676648-66-1 676648-67-2
676648-68-3 676648-69-4 676648-70-7 676648-71-8 676648-72-9
676648-73-0 676648-74-1 676648-75-2 676648-76-3 676648-77-4
676648-78-5 676648-79-6 676648-80-9 676648-81-0 676648-82-1
676648-83-2 676648-84-3 676648-85-4 676648-86-5 676648-87-6
676648-88-7 676648-89-8 676648-90-1 676648-91-2 676648-92-3
676648-93-4 676648-94-5 676648-95-6 676648-96-7 676648-97-8
676648-98-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676648-99-0 676649-00-6 676649-01-7 676649-02-8 676649-03-9
676649-04-0 676649-05-1 676649-06-2 676649-07-3 676649-08-4
676649-09-5 676649-10-8 676649-11-9 676649-12-0 676649-13-1
676649-14-2 676649-15-3 676649-16-4 676649-17-5 676649-18-6
676649-19-7 676649-20-0 676649-21-1 676649-22-2 676649-23-3
676649-24-4 676649-25-5 676649-26-6 676649-27-7 676649-28-8
676649-29-9 676649-30-2 676649-31-3 676649-32-4 676649-33-5
676649-34-6 676649-35-7 676649-36-8 676649-37-9 676649-38-0
676649-39-1 676649-40-4 676649-41-5 676649-42-6 676649-43-7
676649-44-8 676649-45-9 676649-46-0 676649-47-1 676649-48-2
676649-49-3 676649-50-6 676649-51-7 676649-52-8 676649-53-9
676649-54-0 676649-55-1 676649-56-2 676649-57-3 676649-58-4
676649-59-5 676649-60-8 676649-61-9 676649-62-0 676649-63-1
676649-64-2 676649-65-3 676649-66-4 676649-67-5 676649-68-6
676649-69-7 676649-70-0 676649-71-1 676649-72-2 676649-73-3
676649-74-4 676649-75-5 676649-76-6 676649-77-7 676649-78-8
676649-79-9 676649-80-2 676649-81-3 676649-82-4 676649-83-5
676649-84-6 676649-85-7 676649-86-8 676649-87-9 676649-88-0
676649-89-1 676649-90-4 676649-91-5 676649-92-6 676649-93-7
676649-94-8 676649-95-9 676649-96-0 676649-97-1 676649-98-2
676649-99-3 676650-00-3 676650-01-4 676650-02-5 676650-03-6
676650-04-7 676650-05-8 676650-06-9 676650-07-0 676650-08-1
676650-09-2 676650-10-5 676650-11-6 676650-12-7 676650-13-8
676650-14-9 676650-15-0 676650-16-1 676650-17-2 676650-18-3
676650-19-4 676650-20-7 676650-21-8 676650-22-9 676650-23-0
676650-24-1 676650-25-2 676650-26-3 676650-27-4 676650-28-5
676650-29-6 676650-30-9 676650-31-0 676650-32-1 676650-33-2
676650-34-3 676650-35-4 676650-36-5 676650-37-6 676650-38-7
676650-39-8 676650-40-1 676650-41-2 676650-42-3 676650-43-4
676650-44-5 676650-45-6 676650-46-7 676650-47-8 676650-48-9
676650-49-0 676650-50-3 676650-51-4 676650-52-5 676650-53-6
676650-54-7 676650-55-8 676650-56-9 676650-57-0 676650-58-1
676650-59-2 676650-60-5 676650-61-6 676650-62-7 676650-63-8
676650-64-9 676650-65-0 676650-66-1 676650-67-2 676650-68-3
676650-69-4 676650-70-7 676650-71-8 676650-72-9 676650-73-0
676650-74-1 676650-75-2 676650-76-3 676650-77-4 676650-78-5
676650-79-6 676650-80-9 676650-81-0 676650-82-1 676650-83-2
676650-84-3 676650-85-4 676650-86-5 676650-87-6 676650-88-7

676650-89-8 676650-90-1 676650-91-2 676650-92-3 676650-93-4
676650-94-5 676650-95-6 676650-96-7 676650-97-8 676650-98-9
676650-99-0 676651-00-6 676651-01-7 676651-02-8 676651-03-9
676651-04-0 676651-05-1 676651-06-2 676651-07-3 676651-08-4
676651-09-5 676651-10-8 676651-11-9 676651-12-0 676651-13-1
676651-14-2 676651-15-3 676651-16-4 676651-17-5
676651-18-6 676651-19-7 676651-20-0 676651-21-1 676651-22-2
676651-23-3 676651-24-4 676651-25-5 676651-26-6 676651-27-7
676651-28-8 676651-29-9 676651-30-2 676651-31-3 676651-32-4
676651-33-5 676651-34-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676651-35-7 676651-36-8 676651-37-9 676651-38-0 676651-39-1
676651-40-4 676651-41-5 676651-42-6 676651-43-7 676651-44-8
676651-45-9 676651-46-0 676651-47-1 676651-48-2 676651-49-3
676651-50-6 676651-51-7 676651-52-8 676651-53-9 676651-54-0
676651-55-1 676651-56-2 676651-57-3 676651-58-4 676651-59-5
676651-60-8 676651-61-9 676651-62-0 676651-63-1 676651-64-2
676651-65-3 676651-66-4 676651-67-5 676651-68-6 676651-69-7
676651-70-0 676651-71-1 676651-72-2 676651-73-3 676651-74-4
676651-75-5 676651-76-6 676651-77-7 676651-78-8 676651-79-9
676651-80-2 676651-81-3 676651-82-4 676651-83-5 676651-84-6
676651-85-7 676651-86-8 676651-87-9 676651-88-0 676651-89-1
676651-90-4 676651-91-5 676651-92-6 676651-93-7 676651-94-8
676651-95-9 676651-96-0 676651-97-1 676651-98-2 676651-99-3
676652-00-9 676652-01-0 676652-02-1 676652-03-2 676652-04-3
676652-05-4 676652-06-5 676652-07-6 676652-08-7 676652-09-8
676652-10-1 676652-11-2 676652-12-3 676652-13-4 676652-14-5
676652-15-6 676652-16-7 676652-17-8 676652-18-9 676652-19-0
676652-20-3 676652-21-4 676652-22-5 676652-23-6 676652-24-7
676652-25-8 676652-26-9 676652-27-0 676652-28-1 676652-29-2
676652-30-5 676652-31-6 676652-32-7 676652-33-8 676652-34-9
676652-35-0 676652-36-1 676652-37-2 676652-38-3 676652-39-4
676652-40-7 676652-41-8 676652-42-9 676652-43-0 676652-44-1
676652-45-2 676652-46-3 676652-47-4 676652-48-5 676652-49-6
676652-50-9 676652-51-0 676652-52-1 676652-53-2 676652-54-3
676652-55-4 676652-56-5 676652-57-6 676652-58-7 676652-59-8
676652-60-1 676652-61-2 676652-62-3 676652-63-4 676652-64-5
676652-65-6 676652-66-7 676652-67-8 676652-68-9 676652-69-0
676652-70-3 676652-71-4 676652-72-5 676652-73-6 676652-74-7
676652-75-8 676652-76-9 676652-77-0 676652-78-1 676652-79-2
676652-80-5 676652-81-6 676652-82-7 676652-83-8 676652-84-9
676652-85-0 676652-86-1 676652-87-2 676652-88-3 676652-89-4
676652-90-7 676652-91-8 676652-92-9 676652-93-0 676652-94-1
676652-95-2 676652-96-3 676652-97-4 676652-98-5 676652-99-6
676653-00-2 676653-01-3 676653-02-4 676653-03-5 676653-05-7
676653-08-0 676653-09-1 676653-10-4 676653-11-5 676653-12-6
676653-13-7 676653-14-8 676653-15-9 676653-16-0 676653-17-1
676653-18-2 676653-19-3 676653-20-6 676653-21-7 676653-22-8
676653-23-9 676653-24-0 676653-25-1 676653-26-2 676653-27-3
676653-28-4 676653-29-5 676653-30-8 676653-31-9 676653-32-0
676653-33-1 676653-34-2 676653-35-3 676653-36-4 676653-37-5
676653-38-6 676653-39-7 676653-40-0 676653-41-1 676653-42-2
676653-43-3 676653-44-4 676653-45-5 676653-46-6 676653-47-7
676653-48-8 676653-49-9 676653-50-2 676653-51-3 676653-52-4
676653-53-5 676653-54-6 676653-55-7 676653-56-8 676653-57-9
676653-58-0 676653-59-1 676653-60-4 676653-61-5 676653-62-6
676653-63-7 676653-64-8 676653-65-9 676653-66-0 676653-67-1
676653-68-2 676653-69-3 676653-70-6 676653-71-7 676653-72-8
676653-73-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676653-74-0 676653-75-1 676653-76-2 676653-77-3 676653-78-4
676653-79-5 676653-80-8 676653-81-9 676653-82-0 676653-83-1
676653-84-2 676653-85-3 676653-86-4 676653-87-5 676653-88-6
676653-89-7 676653-90-0 676653-91-1 676653-92-2 676653-93-3
676653-94-4 676653-95-5 676653-96-6 676653-97-7 676653-98-8
676653-99-9 676654-00-5 676654-01-6 676654-02-7 676654-03-8
676654-04-9 676654-05-0 676654-06-1 676654-07-2 676654-08-3
676654-09-4 676654-10-7 676654-11-8 676654-12-9 676654-13-0
676654-14-1 676654-15-2 676654-16-3 676654-17-4 676654-18-5
676654-19-6 676654-20-9 676654-21-0 676654-22-1 676654-23-2
676654-24-3 676654-25-4 676654-26-5 676654-27-6 676654-28-7
676654-29-8 676654-30-1 676654-31-2 676654-32-3 676654-33-4
676654-34-5 676654-35-6 676654-36-7 676654-37-8 676654-38-9
676654-39-0 676654-40-3 676654-41-4 676654-42-5 676654-43-6
676654-44-7 676654-45-8 676654-46-9 676654-47-0 676654-48-1
676654-49-2 676654-50-5 676654-51-6 676654-52-7 676654-53-8
676654-54-9 676654-55-0 676654-56-1 676654-57-2 676654-58-3
676654-59-4 676654-60-7 676654-61-8 676654-62-9 676654-63-0
676654-64-1 676654-65-2 676654-66-3 676654-67-4 676654-68-5
676654-69-6 676654-70-9 676654-71-0 676654-72-1 676654-73-2
676654-74-3 676654-75-4 676654-76-5 676654-77-6 676654-78-7
676654-80-1 676654-81-2 676654-82-3 676654-83-4 676654-84-5
676654-85-6 676654-86-7 676654-87-8 676654-88-9 676654-89-0
676654-90-3 676654-91-4 676654-92-5 676654-93-6 676654-94-7
676654-95-8 676654-96-9 676654-97-0 676654-98-1 676654-99-2
676655-00-8 676655-01-9 676655-02-0 676655-03-1 676655-04-2
676655-05-3 676655-06-4 676655-07-5 676655-08-6 676655-09-7
676655-10-0 676655-11-1 676655-12-2 676655-13-3 676655-14-4
676655-15-5 676655-16-6 676655-17-7 676655-18-8 676655-19-9
676655-20-2 676655-21-3 676655-22-4 676655-23-5 676655-24-6
676655-25-7 676655-26-8 676655-27-9 676655-28-0 676655-29-1
676655-30-4 676655-31-5 676655-32-6 676655-33-7 676655-34-8
676655-35-9 676655-36-0 676655-37-1 676655-38-2 676655-39-3
676655-40-6 676655-41-7 676655-42-8 676655-43-9 676655-44-0
676655-45-1 676655-46-2 676655-47-3 676655-48-4 676655-49-5
676655-50-8 676655-51-9 676655-52-0 676655-53-1 676655-54-2
676655-55-3 676655-56-4 676655-57-5 676655-58-6 676655-59-7
676655-60-0 676655-61-1 676655-62-2 676655-63-3 676655-64-4
677000-37-2 677000-38-3 677000-39-4 677000-46-3 677000-47-4
677000-48-5 677000-49-6 677000-53-2 677000-54-3 677000-55-4
677000-56-5 677000-57-6 677000-58-7 677000-59-8 677000-60-1
677000-61-2 677000-62-3 677000-63-4 677000-64-5 677000-65-6
677000-66-7 677000-67-8 677000-68-9 677000-69-0 677000-70-3
677000-71-4 677000-72-5 677000-73-6 677000-74-7 677000-75-8
677000-76-9 677000-77-0 677000-78-1 677000-79-2 677000-80-5
677000-81-6 677000-82-7 677000-83-8 677000-84-9 677000-85-0
677000-86-1 677000-87-2 677000-88-3 677000-89-4 677000-90-7
677000-91-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 677000-92-9 677000-93-0 677000-94-1 677000-95-2 677000-96-3
677000-97-4 677000-98-5 677000-99-6 677001-00-2 677001-01-3
677001-02-4 677001-03-5 677001-04-6 677001-05-7 677001-06-8
677001-07-9 677001-08-0 677001-09-1 677001-10-4 677001-11-5
677001-12-6 677001-13-7 677001-14-8 677001-15-9 677001-16-0
677001-17-1 677001-18-2 677001-19-3 677001-20-6 677001-21-7
677001-22-8 677001-23-9 677001-24-0 677001-25-1 677001-26-2
677001-27-3 677001-28-4 677001-29-5 677001-30-8 677001-31-9
677001-32-0 677001-33-1 677001-34-2 677001-35-3 677001-36-4
677001-37-5 677001-38-6 677001-39-7 677001-40-0 677001-41-1
677001-42-2 677001-43-3 677001-44-4 677001-45-5 677001-46-6
677001-47-7 677001-48-8 677001-49-9 677001-51-3 677001-53-5
677001-55-7 677001-56-8 677001-58-0 677001-60-4 677001-62-6
677001-63-7 677001-64-8 677001-65-9 677001-66-0 677001-67-1

677001-68-2 677001-69-3 677001-70-6 677001-71-7 677001-72-8
677001-73-9 677001-74-0 677001-75-1 677001-76-2 677001-77-3
677001-78-4 677001-79-5 677001-80-8 677001-81-9 677001-82-0
677001-83-1 677001-84-2 677001-85-3 677001-86-4 677001-87-5
677001-88-6 677001-89-7 677001-90-0 677001-91-1 677001-92-2
677001-93-3 677001-94-4 677001-95-5 677001-96-6 677001-97-7
677001-98-8 677001-99-9 677002-00-5 677002-01-6 677002-02-7
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

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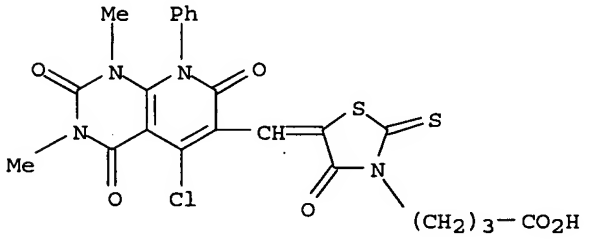
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 59-05-2, Methotrexate 302-79-4, Tretinoin 10540-29-1, Tamoxifen 33069-62-4, Paclitaxel 114977-28-5, Docetaxel 174722-31-7, Rituximab
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)

IT 676651-16-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

RN 676651-16-4 HCAPLUS

CN 3-Thiazolidinebutanoic acid, 5-[(5-chloro-1,2,3,4,7,8-hexahydro-1,3-dimethyl-2,4,7-trioxo-8-phenylpyrido[2,3-d]pyrimidin-6-yl)methylene]-4-oxo-2-thioxo- (9CI) (CA INDEX NAME)



L59 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:291950 HCAPLUS

DN 140:315042

ED Entered STN: 09 Apr 2004

TI Pin1-modulating compounds and methods of use for the treatment of Pin1-associated diseases, including cancer

IN Mckee, Timothy D.; Suto, Robert K.; Tibbitts, Thomas; Sowadski, Janusz

PA Pintex Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 166 pp.
CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K031-41
ICS A61K031-425

CC 1-6 (Pharmacology)
Section cross-reference(s): 27, 28

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004028535	A1	20040408	WO 2003-US6675	20030303 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004214872	A1	20041028	US 2003-379408	20030303 <--
PRAI	US 2002-414077P	P	20020926 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004028535	ICM	A61K031-41
	ICS	A61K031-425
WO 2004028535	ECLA	A61K031/41; A61K031/425 <--
US 2004214872	NCL	514/369.000
	ECLA	A61K031/41; A61K031/425 <--

OS MARPAT 140:315042

AB The invention is directed to modulators, e.g., inhibitors, of Pin1 and Pin1-related proteins and the use of such modulators for treatment of Pin1 associated states, e.g., for the treatment of cancer. Synthetic methods are included.

ST Pin1 modulator therapeutic cancer treatment

IT Cyclins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(D1; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Skin
(Merkel cell, cancer; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Adrenal gland, neoplasm
Antitumor agents
Drug delivery systems
Esophagus, neoplasm
Hodgkin's disease
Human
Lymphoma
Mammary gland, neoplasm
Melanoma
Mouth, neoplasm
Neoplasm
Ovary, neoplasm
Pheochromocytoma
Prostate gland, neoplasm
Sarcoma
Testis, neoplasm
Transformation, neoplastic
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Transforming proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Aldehydes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Radiotherapy
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)

IT Interleukin 2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)

IT Esophagus, neoplasm
Gallbladder, neoplasm
Lung, neoplasm
Pancreas, neoplasm
Parathyroid gland, neoplasm
Stomach, neoplasm
(adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Adrenal gland, neoplasm
(adenoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Adenoma
(adrenal; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm
(astrocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Skin, neoplasm
(basolioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(bladder transitional cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Sarcoma
(carcinosarcoma, uterus; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(carcinosarcoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(cervix, carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(cervix; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(colon adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon, adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon, adenoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(colon; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adenoma
(colonic; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(cutaneous squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT DNA
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(damage; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(endometrial; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(endometrioid; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Uterus, neoplasm
(endometrium, carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(esophageal adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(follicular and adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(gastric adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm
(glioblastoma; Pin1-modulating compds. for treatment of Pin1-associated

diseases, including cancer)
IT Carcinoma
(hepatocellular; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Liver, neoplasm
(hepatoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Hyperplasia
(inhibitors; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)
IT Lung, neoplasm
(large cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adipose tissue, neoplasm
(lipoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Adipose tissue, neoplasm
Sarcoma
(liposarcoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(medullary carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lymphoma
(mucosa-associated lymphoid tissue; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Astrocyte
(neoplasm, astrocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Oligodendrocyte
(neoplasm, oligodendroglioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Skin, disease
(nevus; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lymphoma
(non-Hodgkin's; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Neuroglia, neoplasm
(oligodendroglioma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Kidney, neoplasm
(oncocytoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Ras proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(p21c-Ha-ras; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pancreatic adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thyroid gland, neoplasm
(papillary carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary small-cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(pulmonary squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Kidney, neoplasm
(renal cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT Carcinoma
(renal cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Testis, neoplasm
(seminoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Intestine, neoplasm
(small, adenocarcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lung, neoplasm
(small-cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Lung, neoplasm
Skin, neoplasm
Skin, neoplasm
(squamous cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(squamous cell; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Thymus gland, neoplasm
(thymoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(thyroid medullary; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Carcinoma
(thyroid papillary; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT Bladder, neoplasm
(transitional cell carcinoma; Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT 415965-81-0, Prolyl isomerase Pin1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)
IT 536-17-4 3785-78-2 4649-06-3 4703-96-2 6594-02-1 7025-19-6
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

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433246-32-3 433254-12-7 438244-17-8 442554-46-3 461715-64-0
461715-66-2 461715-77-5 464902-22-5 473390-72-6 476292-76-9
476292-81-6 489423-55-4 518349-54-7 519012-18-1 551922-52-2
590363-34-1 591224-27-0 591224-36-1 591224-53-2 591224-63-4
607705-42-0 609832-71-5 609833-33-2 609833-83-2 609833-90-1
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612804-35-0 612804-36-1 612804-38-3 612804-39-4 612804-66-7
612804-67-8 612804-69-0 612804-71-4 612804-79-2 612804-82-7
612804-83-8 612804-84-9 613224-41-2 613224-43-4 618077-52-4
620574-90-5 629606-31-1 629607-19-8 629607-20-1 629608-14-6
629608-15-7 629608-78-2 630047-84-6 634577-58-5 634578-58-8
634579-63-8 634579-64-9 641997-85-5 676643-15-5 676643-18-8
676643-37-1 676643-41-7 676643-46-2 676643-47-3 676643-48-4
676643-49-5 676643-51-9 676643-54-2 676643-56-4 676643-57-5
676643-59-7 676643-64-4 676643-66-6 676643-68-8 676643-69-9
676643-72-4 676643-74-6 676643-75-7 676643-76-8 676643-78-0
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676644-30-7 676644-32-9 676644-36-3 676644-38-5 676644-40-9
676644-41-0 676644-43-2 676644-49-8 676644-50-1 676644-52-3
676644-56-7 676644-58-9 676644-63-6 676644-69-2 676644-71-6
676644-75-0 676644-79-4 676644-83-0 676644-85-2 676644-86-3
676644-88-5 676644-91-0 676644-95-4 676644-99-8 676645-01-5

676645-03-7 676645-06-0 676645-09-3 676645-13-9 676645-18-4
676645-20-8 676645-21-9 676645-23-1 676645-24-2 676645-40-2
676645-50-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676645-55-9 676645-56-0 676645-58-2 676645-60-6 676645-62-8
676645-64-0 676645-66-2 676645-67-3 676645-69-5 676645-70-8
676645-71-9 676645-74-2 676645-79-7 676645-81-1 676645-82-2
676645-83-3 676645-85-5 676645-86-6 676645-90-2 676645-92-4
676645-94-6 676646-07-4 676646-20-1 676646-26-7 676646-27-8
676646-28-9 676646-30-3 676646-32-5 676646-34-7 676646-37-0
676646-39-2 676646-41-6 676646-42-7 676646-44-9 676646-46-1
676646-48-3 676646-50-7 676646-52-9 676646-53-0 676646-54-1
676646-56-3 676646-58-5 676646-60-9 676646-61-0 676646-62-1
676646-63-2 676646-64-3 676646-65-4 676646-70-1 676646-72-3
676646-74-5 676646-76-7 676646-78-9 676646-80-3 676646-81-4
676646-83-6 676646-85-8 676646-86-9 676646-88-1 676646-90-5
676646-92-7 676646-94-9 676646-95-0 676646-96-1 676646-97-2
676646-98-3 676646-99-4 676647-00-0 676647-01-1 676647-02-2
676647-03-3 676647-04-4 676647-05-5 676647-06-6 676647-07-7
676647-08-8 676647-09-9 676647-10-2 676647-11-3 676647-12-4
676647-13-5 676647-14-6 676647-15-7 676647-16-8 676647-17-9
676647-18-0 676647-19-1 676647-20-4 676647-21-5 676647-22-6
676647-23-7 676647-24-8 676647-25-9 676647-26-0 676647-28-2
676647-29-3 676647-31-7 676647-32-8 676647-33-9 676647-34-0
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676647-81-7 676647-82-8 676647-84-0 676647-86-2 676647-87-3
676647-88-4 676647-89-5 676647-90-8 676647-91-9 676647-92-0
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676647-98-6 676647-99-7 676648-00-3 676648-01-4 676648-02-5
676648-03-6 676648-04-7 676648-05-8 676648-06-9 676648-07-0
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676648-13-8 676648-14-9 676648-15-0 676648-16-1 676648-17-2
676648-18-3 676648-19-4 676648-20-7 676648-21-8 676648-22-9
676648-23-0 676648-24-1 676648-25-2 676648-26-3 676648-27-4
676648-28-5 676648-29-6 676648-30-9 676648-31-0 676648-32-1
676648-33-2 676648-34-3 676648-35-4 676648-36-5 676648-37-6
676648-38-7 676648-39-8 676648-40-1 676648-41-2 676648-42-3
676648-43-4 676648-44-5 676648-45-6 676648-46-7 676648-47-8
676648-48-9 676648-49-0 676648-50-3 676648-51-4 676648-52-5
676648-53-6 676648-54-7 676648-55-8 676648-56-9 676648-57-0
676648-58-1 676648-59-2 676648-60-5 676648-61-6 676648-62-7
676648-63-8 676648-64-9 676648-65-0 676648-66-1 676648-67-2
676648-68-3 676648-69-4 676648-70-7 676648-71-8 676648-72-9
676648-73-0 676648-74-1 676648-75-2 676648-76-3 676648-77-4
676648-78-5 676648-79-6 676648-80-9 676648-81-0 676648-82-1
676648-83-2 676648-84-3 676648-85-4 676648-86-5 676648-87-6
676648-88-7 676648-89-8 676648-90-1 676648-91-2 676648-92-3
676648-93-4 676648-94-5 676648-95-6 676648-96-7 676648-97-8
676648-98-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676648-99-0 676649-00-6 676649-01-7 676649-02-8 676649-03-9
676649-04-0 676649-05-1 676649-06-2 676649-07-3 676649-08-4
676649-09-5 676649-10-8 676649-11-9 676649-12-0 676649-13-1
676649-14-2 676649-15-3 676649-16-4 676649-17-5 676649-18-6
676649-19-7 676649-20-0 676649-21-1 676649-22-2 676649-23-3
676649-24-4 676649-25-5 676649-26-6 676649-27-7 676649-28-8
676649-29-9 676649-30-2 676649-31-3 676649-32-4 676649-33-5

676649-34-6 676649-35-7 676649-36-8 676649-37-9 676649-38-0
676649-39-1 676649-40-4 676649-41-5 676649-42-6 676649-43-7
676649-44-8 676649-45-9 676649-46-0 676649-47-1 676649-48-2
676649-49-3 676649-50-6 676649-51-7 676649-52-8 676649-53-9
676649-54-0 676649-55-1 676649-56-2 676649-57-3 676649-58-4
676649-59-5 676649-60-8 676649-61-9 676649-62-0 676649-63-1
676649-64-2 676649-65-3 676649-66-4 676649-67-5 676649-68-6
676649-69-7 676649-70-0 676649-71-1 676649-72-2 676649-73-3
676649-74-4 676649-75-5 676649-76-6 676649-77-7 676649-78-8
676649-79-9 676649-80-2 676649-81-3 676649-82-4 676649-83-5
676649-84-6 676649-85-7 676649-86-8 676649-87-9 676649-88-0
676649-89-1 676649-90-4 676649-91-5 676649-92-6 676649-93-7
676649-94-8 676649-95-9 676649-96-0 676649-97-1 676649-98-2
676649-99-3 676650-00-3 676650-01-4 676650-02-5 676650-03-6
676650-04-7 676650-05-8 676650-06-9 676650-07-0 676650-08-1
676650-09-2 676650-10-5 676650-11-6 676650-12-7 676650-13-8
676650-14-9 676650-15-0 676650-16-1 676650-17-2 676650-18-3
676650-19-4 676650-20-7 676650-21-8 676650-22-9 676650-23-0
676650-24-1 676650-25-2 676650-26-3 676650-27-4 676650-28-5
676650-29-6 676650-30-9 676650-31-0 676650-32-1 676650-33-2
676650-34-3 676650-35-4 676650-36-5 676650-37-6 676650-38-7
676650-39-8 676650-40-1 676650-41-2 676650-42-3 676650-43-4
676650-44-5 676650-45-6 676650-46-7 676650-47-8 676650-48-9
676650-49-0 676650-50-3 676650-51-4 676650-52-5 676650-53-6
676650-54-7 676650-55-8 676650-56-9 676650-57-0 676650-58-1
676650-59-2 676650-60-5 676650-61-6 676650-62-7 676650-63-8
676650-64-9 676650-65-0 676650-66-1 676650-67-2 676650-68-3
676650-69-4 676650-70-7 676650-71-8 676650-72-9 676650-73-0
676650-74-1 676650-75-2 676650-76-3 676650-77-4 676650-78-5
676650-79-6 676650-80-9 676650-81-0 676650-82-1 676650-83-2
676650-84-3 676650-85-4 676650-86-5 676650-87-6 676650-88-7
676650-89-8 676650-90-1 676650-91-2 676650-92-3 676650-93-4
676650-94-5 676650-95-6 676650-96-7 676650-97-8 676650-98-9
676650-99-0 676651-00-6 676651-01-7 676651-02-8 676651-03-9
676651-04-0 676651-05-1 676651-06-2 676651-07-3 676651-08-4
676651-09-5 676651-10-8 676651-11-9 676651-12-0 676651-13-1
676651-14-2 676651-15-3 676651-16-4 676651-17-5
676651-18-6 676651-19-7 676651-20-0 676651-21-1 676651-22-2
676651-23-3 676651-24-4 676651-25-5 676651-26-6 676651-27-7
676651-28-8 676651-29-9 676651-30-2 676651-31-3 676651-32-4
676651-33-5 676651-34-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676651-35-7 676651-36-8 676651-37-9 676651-38-0 676651-39-1
676651-40-4 676651-41-5 676651-42-6 676651-43-7 676651-44-8
676651-45-9 676651-46-0 676651-47-1 676651-48-2 676651-49-3
676651-50-6 676651-51-7 676651-52-8 676651-53-9 676651-54-0
676651-55-1 676651-56-2 676651-57-3 676651-58-4 676651-59-5
676651-60-8 676651-61-9 676651-62-0 676651-63-1 676651-64-2
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676651-70-0 676651-71-1 676651-72-2 676651-73-3 676651-74-4
676651-75-5 676651-76-6 676651-77-7 676651-78-8 676651-79-9
676651-80-2 676651-81-3 676651-82-4 676651-83-5 676651-84-6
676651-85-7 676651-86-8 676651-87-9 676651-88-0 676651-89-1
676651-90-4 676651-91-5 676651-92-6 676651-93-7 676651-94-8
676651-95-9 676651-96-0 676651-97-1 676651-98-2 676651-99-3
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676652-15-6 676652-16-7 676652-17-8 676652-18-9 676652-19-0
676652-20-3 676652-21-4 676652-22-5 676652-23-6 676652-24-7
676652-25-8 676652-26-9 676652-27-0 676652-28-1 676652-29-2
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676652-50-9 676652-51-0 676652-52-1 676652-53-2 676652-54-3
676652-55-4 676652-56-5 676652-57-6 676652-58-7 676652-59-8
676652-60-1 676652-61-2 676652-62-3 676652-63-4 676652-64-5
676652-65-6 676652-66-7 676652-67-8 676652-68-9 676652-69-0
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676652-75-8 676652-76-9 676652-77-0 676652-78-1 676652-79-2
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676652-85-0 676652-86-1 676652-87-2 676652-88-3 676652-89-4
676652-90-7 676652-91-8 676652-92-9 676652-93-0 676652-94-1
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676653-18-2 676653-19-3 676653-20-6 676653-21-7 676653-22-8
676653-23-9 676653-24-0 676653-25-1 676653-26-2 676653-27-3
676653-28-4 676653-29-5 676653-30-8 676653-31-9 676653-32-0
676653-33-1 676653-34-2 676653-35-3 676653-36-4 676653-37-5
676653-38-6 676653-39-7 676653-40-0 676653-41-1 676653-42-2
676653-43-3 676653-44-4 676653-45-5 676653-46-6 676653-47-7
676653-48-8 676653-49-9 676653-50-2 676653-51-3 676653-52-4
676653-53-5 676653-54-6 676653-55-7 676653-56-8 676653-57-9
676653-58-0 676653-59-1 676653-60-4 676653-61-5 676653-62-6
676653-63-7 676653-64-8 676653-65-9 676653-66-0 676653-67-1
676653-68-2 676653-69-3 676653-70-6 676653-71-7 676653-72-8
676653-73-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 676653-74-0 676653-75-1 676653-76-2 676653-77-3 676653-78-4
676653-79-5 676653-80-8 676653-81-9 676653-82-0 676653-83-1
676653-84-2 676653-85-3 676653-86-4 676653-87-5 676653-88-6
676653-89-7 676653-90-0 676653-91-1 676653-92-2 676653-93-3
676653-94-4 676653-95-5 676653-96-6 676653-97-7 676653-98-8
676653-99-9 676654-00-5 676654-01-6 676654-02-7 676654-03-8
676654-04-9 676654-05-0 676654-06-1 676654-07-2 676654-08-3
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676654-14-1 676654-15-2 676654-16-3 676654-17-4 676654-18-5
676654-19-6 676654-20-9 676654-21-0 676654-22-1 676654-23-2
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676654-39-0 676654-40-3 676654-41-4 676654-42-5 676654-43-6
676654-44-7 676654-45-8 676654-46-9 676654-47-0 676654-48-1
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676654-54-9 676654-55-0 676654-56-1 676654-57-2 676654-58-3
676654-59-4 676654-60-7 676654-61-8 676654-62-9 676654-63-0
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676654-69-6 676654-70-9 676654-71-0 676654-72-1 676654-73-2
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676654-90-3 676654-91-4 676654-92-5 676654-93-6 676654-94-7
676654-95-8 676654-96-9 676654-97-0 676654-98-1 676654-99-2
676655-00-8 676655-01-9 676655-02-0 676655-03-1 676655-04-2
676655-05-3 676655-06-4 676655-07-5 676655-08-6 676655-09-7
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676655-55-3 676655-56-4 676655-57-5 676655-58-6 676655-59-7
676655-60-0 676655-61-1 676655-62-2 676655-63-3 676655-64-4
677000-37-2 677000-38-3 677000-39-4 677000-46-3 677000-47-4
677000-48-5 677000-49-6 677000-53-2 677000-54-3 677000-55-4
677000-56-5 677000-57-6 677000-58-7 677000-59-8 677000-60-1
677000-61-2 677000-62-3 677000-63-4 677000-64-5 677000-65-6
677000-66-7 677000-67-8 677000-68-9 677000-69-0 677000-70-3
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677000-81-6 677000-82-7 677000-83-8 677000-84-9 677000-85-0
677000-86-1 677000-87-2 677000-88-3 677000-89-4 677000-90-7
677000-91-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 677000-92-9 677000-93-0 677000-94-1 677000-95-2 677000-96-3
677000-97-4 677000-98-5 677000-99-6 677001-00-2 677001-01-3
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677001-32-0 677001-33-1 677001-34-2 677001-35-3 677001-36-4
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677003-40-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 677003-41-7 677003-42-8 677003-43-9 677003-44-0 677003-45-1
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677004-86-3 677004-87-4 677004-88-5 677004-91-0 677004-92-1
677004-93-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 79-08-3, Bromoacetic acid 98-80-6, Phenylboronic acid 141-84-4, Rhodanine 1899-24-7, 5-Bromo-2-furaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

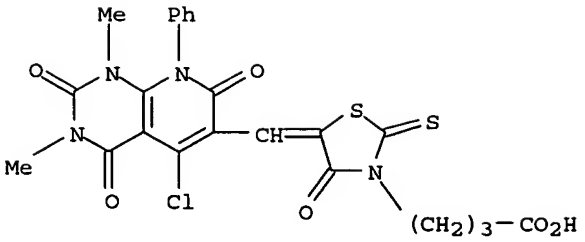
IT 303790-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

IT 59-05-2, Methotrexate 302-79-4, Tretinoin 10540-29-1, Tamoxifen 33069-62-4, Paclitaxel 114977-28-5, Docetaxel 174722-31-7, Rituximab
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer, and use with other agents)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) F Hoffmann-La Roche; WO 0157006 A1 2001 HCAPLUS
(2) Geron Corporation; WO 0102377 A1 2001 HCAPLUS

IT **676651-16-4**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

RN 676651-16-4 HCAPLUS
CN 3-Thiazolidinebutanoic acid, 5-[(5-chloro-1,2,3,4,7,8-hexahydro-1,3-dimethyl-2,4,7-trioxo-8-phenylpyrido[2,3-d]pyrimidin-6-yl)methylene]-4-oxo-2-thioxo- (9CI) (CA INDEX NAME)



L59 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:120960 HCAPLUS
DN 140:181711
ED Entered STN: 13 Feb 2004
TI Preparation of bicyclo[4.2.1]nonane nucleoside analogs for the treatment of Flaviviridae infections
IN Wang, Peiyuan; Stuyver, Lieven J.; Watanabe, Kyoichi A.; Hassan, Abdalla; Chun, Byoung-Known; Hollecker, Laurent
PA Pharmasset, Ltd., Barbados
SO PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C12N
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
FAN.CNT 2

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PI	WO 2004013300	A2	20040212	WO 2003-US24324	20030801 <--
	WO 2004013300	A3	20040923		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	US 2004067877	A1	20040408	US 2003-632875	20030801 <--
	US 2004082574	A1	20040429	US 2003-632997	20030801 <--
	EP 1545545	A2	20050629	EP 2003-767138	20030801 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRAI	US 2002-453716P	P	20020801 <--		
	US 2002-453715P	P	20020801 <--		
	WO 2003-US24324	W	20030801		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004013300	ICM	C12N
WO 2004013300	ECLA	A61K031/513; A61K031/513+M; A61K031/553; A61K031/553+M; A61K031/58; A61K031/58+M; A61K031/7056+M; A61K031/7068; A61K031/7068+M; A61K031/7072; A61K031/7072+M; A61K038/20K+M; A61K038/21+M; C07D487/16+249C+243D+239C; C07D498/22+307C+273D+249C+239C; C07D498/22+317B+307C+273D+249C+239C <--
US 2004067877	NCL	514/008.000; 514/269.000; 514/050.000; 514/176.000
	ECLA	A61K031/513; A61K031/513+M; A61K031/553; A61K031/553+M; A61K031/58; A61K031/58+M; A61K031/7068; A61K031/7068+M;

A61K031/7072; A61K031/7072+M; A61K038/20K+M;
A61K038/21+M; C07H019/06 <--
US 2004082574 NCL 514/221.000
ECLA A61K031/513; A61K031/513+M; A61K031/553; A61K031/553+M;
A61K031/58; A61K031/58+M; A61K031/7068; A61K031/7068+M;
A61K031/7072; A61K031/7072+M; A61K038/20K+M;
A61K038/21+M; C07D487/16+249C+243D+239C;
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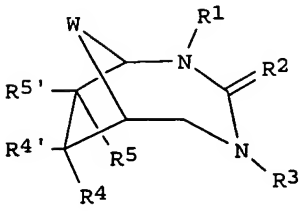
OS MARPAT 140:181711
GI



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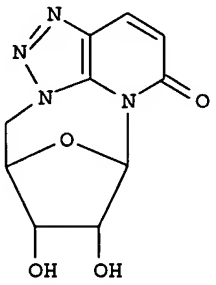

II

AB The disclosed invention is a bicyclo[4.2.1]nonane nucleoside analogs I, wherein R1 is hydrogen, lower alkyl, alkylene, alkenyl, carbocycle, aryl, heterocycle, heteroaryl, aralkyl, aminoalkyl, aminoaryl or aminoacyl of C1-C6; R2 is oxygen, sulfur, -NR' or -CR'2, wherein each R' is independently H, lower alkyl, alkylene, alkenyl, aryl, or aralkyl of C1-C6; R3 is H, lower alkyl, alkylene, alkenyl, carbocycle, aryl, heterocycle, heteroaryl, aralkyl, aminoalkyl, aminoaryl or aminoacyl of C1-C6; each R4, R4', R5, and R5' is independently H, halogen, pseudo-halogen, CN, NO2, lower alkyl of C1-C6, halogenated lower alkyl, hydroxy, alkoxy, CH2OH, CH2OR6, NH2, -NR6R7, or a residue of an amino acid; wherein at least one of R4 and R4' is H; each R6 and R7 is independently H, alkyl, halogenated alkyl, alkylene, alkenyl, carbocycle, aryl, heterocycle, heteroaryl, aralkyl, or acyl; and its pharmaceutically acceptable salt or prodrug, and its composition and method of use to treat Flaviviridae (Hepacivirus, Flavivirus, and Pestivirus) infections on a host, including animals, and especially humans. Thus, nucleoside analog II was prepared and administered at 5 mg/kg/day QD to chronically infected chimpanzees resulted in a significant reduction in viral load at day 4 and no change in hematol. or blood chemical parameters was observed

ST human antiviral nucleoside bicyclononane Flaviviridae prepn interferon

IT Antiviral agents
Human
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

IT Interleukin 10
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

IT Nucleosides, preparation
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

IT Drug delivery systems
(prodrugs; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

IT Infection
(viral; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT Interferons
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT Interferons
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT Interferons
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT Interferons
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ω; preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT 56-92-8, Histamine dihydrochloride 768-94-5, AMANTADINE 36791-04-5, Ribavirin 62304-98-7, ZADAXIN 119567-79-2, VIRAMIDINE 198153-51-4, PEGASYS 206269-27-4, LEVOVIRIN 220581-49-7, REBIF 223603-41-6, ISIS 14803 402957-28-2, VX 950 472960-22-8, ALBUFERON 624747-15-5, IDN-6556
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT 656808-44-5P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT 10380-93-5P 57901-65-2P 57901-66-3P 150938-54-8P 656808-42-3P
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656809-73-3P **656809-79-9P** 656809-80-2P 656809-81-3P
656809-82-4P 656809-83-5P 656809-84-6P 656809-85-7P 657394-45-1P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT 3080-30-6P 15083-05-3P 17044-78-9P 19556-62-8P 29617-86-5P
51172-83-9P 54503-61-6P 57071-82-6P 57901-59-4P 57901-63-0P
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656809-72-2P 656809-74-4P 656809-75-5P **656809-76-6P**
656809-77-7P **656809-78-8P** 657394-44-0P 657394-48-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)
IT 58-96-8, Uridine 107-20-0, Chloroacetaldehyde 403-43-0 593-56-6
873-83-6 957-75-5 4137-57-9 5418-51-9 6160-65-2 6723-30-4
6974-32-9 24259-59-4, L-Ribose 31458-45-4 76222-39-4 415704-30-2

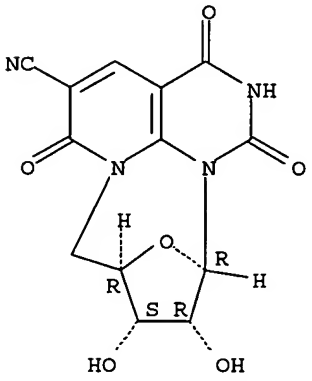
656808-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

IT 656809-79-9P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

RN 656809-79-9 HCAPLUS

CN 8,11-Epoxy-1H,6H,7H-2,6a,11a-triazacycloocta[de]naphthalene-5-carbonitrile, 2,3,8,9,10,11-hexahydro-9,10-dihydroxy-1,3,6-trioxo-, (8R,9S,10R,11R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

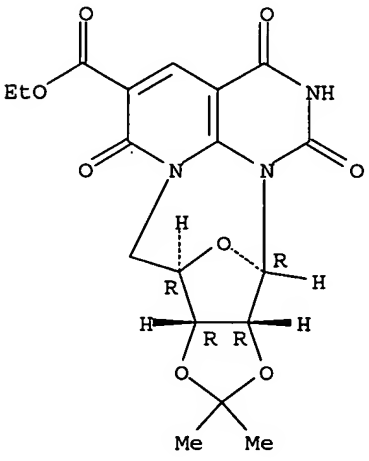


IT 656809-76-6P 656809-77-7P 656809-78-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclo..nonane nucleoside analogs for the treatment of flaviviridae infections)

RN 656809-76-6 HCAPLUS

CN 8,12-Epoxy-1H,6H,7H-9,11-dioxa-2,6a,12a-triazacyclopenta[5,6]cycloocta[1,2,3-de]naphthalene-5-carboxylic acid, 2,3,8,8a,11a,12-hexahydro-10,10-dimethyl-1,3,6-trioxo-, ethyl ester, (8R,8aR,11aR,12R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 656809-77-7 HCAPLUS
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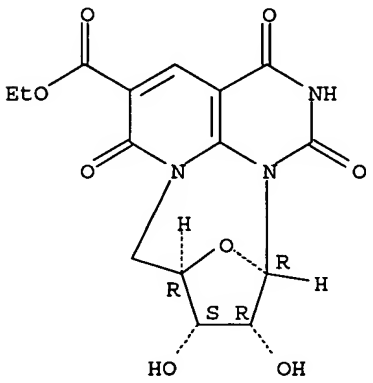
Absolute stereochemistry.



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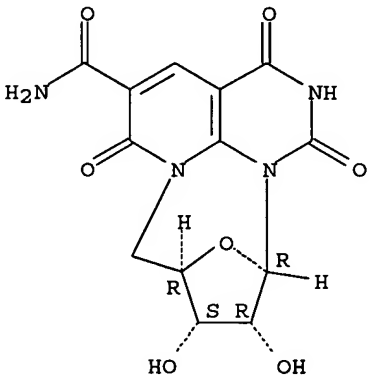
CN 8,11-Epoxy-1H,6H,7H-2,6a,11a-triazacycloocta[de]naphthalene-5-carboxamide, 2,3,8,9,10,11-hexahydro-9,10-dihydroxy-1,3,6-trioxo-, (8R,9S,10R,11R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:798959 HCAPLUS
DN 139:286330
ED Entered STN: 13 Oct 2003
TI Pin1-modulating compounds and methods of use thereof
IN Mckee, Timothy D.; Suto, Robert K.; Tibbitts, Thomas; Sowadski, Janusz
PA Pintex Pharmaceutical, Inc., USA
SO PCT Int. Appl., 230 pp.
CODEN: PIXXD2
DT Patent
LA English
IC C07D239-62; C07D239-66; C07D473-08; C07D475-14; C07D487-04; A61K031-515; A61K031-52; A71K031-525
CC 1-6 (Pharmacology)
Section cross-reference(s): 28
FAN.CNT 2

Search done by Noble Jarrell

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PRAI	US 2002-361246P	P	20020301 <--		
	WO 2003-US6674	A	20030303		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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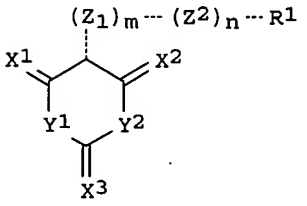
WO 2003074497	ECLA	A61K031/515; A61K031/52; A61K031/525; C07D405/06+307B+239B <--

GI



I

AB The invention is directed to modulators, e.g., inhibitors, of Pin 1 and Pin 1-related proteins and the use of such modulators for treatment of Pin 1 associated states, e.g., for the treatment of cancer. This method includes administering to the subject an effective amount of a Pin1-modulating compound of formula I (the dashed line to R1 indicates a single or a double bond; n or m are independently 0 or 1; X1, X2, and X3 are each independently O, S, or NR2; Y1, and Y2 are each independently O, S, or NR3; R1, R2 and R3 are each independently substituted or unsubstituted alkyl, alkenyl, alkynyl, aryl, hydrogen, acyl, or any combination thereof; Z1 and Z2 are each independently CH2, CH, or N). In a second embodiment, the invention pertains, at least in part, to a method for treating cyclin D1 overexpression in a subject. [This abstract record is two of two records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.].

ST pin1 modulator cancer treatment cyclin D1 overexpression

IT Cyclins

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(D1; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Adrenal gland, neoplasm
Antitumor agents
Bladder, neoplasm
Esophagus, neoplasm
Gallbladder, neoplasm
Hodgkin's disease
Human
Hyperplasia
Intestine, neoplasm
Kidney, neoplasm
Lung, neoplasm
Lymphoma
Mammary gland, neoplasm
Melanoma
Mouth, neoplasm
Neoplasm
Pancreas, neoplasm
Parathyroid gland, neoplasm
Pheochromocytoma
Prostate gland, neoplasm
Radiotherapy
Sarcoma
Skin, neoplasm
Stomach, neoplasm
Testis, neoplasm
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Interleukin 2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Neuroglia, neoplasm
(astrocytoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Thyroid gland, neoplasm
(carcinoma, adenocarcinoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Uterus, neoplasm
(cervix, carcinoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Carcinoma
(cervix; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Intestine, neoplasm
(colon; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT DNA
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(damage; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Thyroid gland, neoplasm
(follicular cell carcinoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT Neuroglia, neoplasm
(glioblastoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Carcinoma
(hepatocellular; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Liver, neoplasm
(hepatoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Adipose tissue, neoplasm
Sarcoma
(liposarcoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Astrocyte
(neoplasm, astrocytoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Oligodendrocyte
(neoplasm, oligodendroglioma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Neuroglia, neoplasm
(oligodendroglioma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Gene, animal
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(oncogene, expression; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Ras proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(p21Ha-ras; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Intestine, neoplasm
(small; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Thymus gland, neoplasm
(thymoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
IT Carcinoma
(thyroid follicular cell; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
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(thyroid, adenocarcinoma; Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

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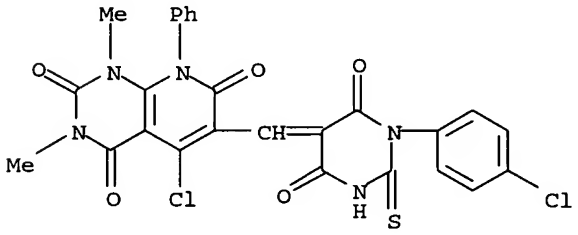
609840-77-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

IT 609836-33-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Pin1-modulating compds. for treatment of disease states such as cancer in combination with other agents in relation to cyclin D1 overexpression)

RN 609836-33-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-chloro-6-[[1-(4-chlorophenyl)tetrahydro-4,6-dioxo-2-thioxo-5(2H)-pyrimidinylidene]methyl]-1,3-dimethyl-8-phenyl- (9CI) (CA INDEX NAME)



L59 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:487577 HCAPLUS
DN 137:63420
ED Entered STN: 28 Jun 2002
TI Preparation of lactone ketolide macrolide erythromycin antibiotics
IN Andreotti, Daniele; Arista, Luca; Biondi, Stefano; Cardullo, Francesca; Damiani, Frederica; Lociuro, Sergio; Marchioro, Carla; Merlo, Giancarlo; Mingardi, Anna; Niccolai, Daniela; Paio, Alfredo; Piga, Elisabetta; Pozzan, Alfonso; Seri, Catia; Tarsi, Luca; Terreni, Silvia; Tibasco, Jessica
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 215 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07H017-08
ICS A61K031-70
CC 33-7 (Carbohydrates)
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002050091	A1	20020627	WO 2001-GB5665	20011220 <--
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	AU 2002017277	A5	20020701	AU 2002-17277	20011220 <--
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	ZA 2003004748	A	20040423	ZA 2003-4748	20030619 <--
	NO 2003002846	A	20030820	NO 2003-2846	20030620 <--
	US 2004077557	A1	20040422	US 2003-450893	20031119 <--
PRAI	GB 2000-31309	A	20001221 <--		
	GB 2001-26276	A	20011101 <--		
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002050091	ICM	C07H017-08
	ICS	A61K031-70
WO 2002050091	ECLA	A61K031/70R5L; C07H017/08F <--
JP 2004531471	FTERM	4C057/AA03; 4C057/AA18; 4C057/KK13; 4C086/AA01; 4C086/AA02; 4C086/AA03; 4C086/AA04; 4C086/EA13; 4C086/MA01; 4C086/NA05; 4C086/ZB35 <--
US 2004077557	NCL	514/028.000; 536/007.100
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OS MARPAT 137:63420

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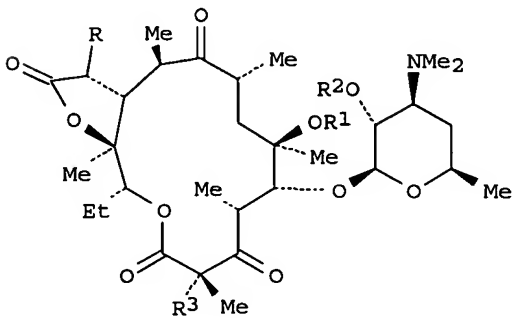

I

AB The present invention relates to lactone ketolides I wherein R is H, CN, substituted alkyl; R1 is alkyl, alkenyl; R2 is H, hydroxy protecting group; R3 is H, halogen, and pharmaceutically acceptable salts and solvates thereof, to process for their preparation and their use in therapy or prophylaxis of systemic or topical bacterial infections in a human or animal body. Thus, (11S,21R)-3-decladinosyl-11,12-dideoxy-6-O-methyl-3-oxo-12,11-[oxycarbonyl-(cyano)-methylene]erythromycin A was prepared and tested as antibacterial agent against Streptococcus pneumoniae and Streptococcus pyogenes (MIC ≤ 1 μg/mL).

ST therapy prophylaxis systemic bacterial infection human erythromycin prepn pyogenes; macrolide antibiotic human antibacterial lactone ketolide prepn Streptococcus pneumoniae

IT Infection
(bacterial; preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT Antibiotics
(macrolide; preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT Antibacterial agents
Antibiotics
Human
Streptococcus pneumoniae
Streptococcus pyogenes
Therapy
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 439099-89-5P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

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RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

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439105-01-8P 439105-02-9P 439105-03-0P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and

their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 439105-04-1P 439105-05-2P 439105-06-3P 439105-07-4P 439105-08-5P
439105-09-6P 439105-10-9P 439105-11-0P 439105-12-1P 439105-13-2P
439105-14-3P 439105-15-4P 439105-16-5P 439105-17-6P 439105-18-7P
439105-19-8P 439105-20-1P 439105-21-2P 439105-22-3P 439105-23-4P
439105-24-5P 439105-25-6P 439105-26-7P 439105-27-8P 439105-28-9P
439105-29-0P 439105-30-3P 439105-31-4P 439105-32-5P 439105-33-6P
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439105-44-9P 439105-45-0P 439105-46-1P 439105-47-2P 439105-48-3P
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439124-94-4P 439124-96-6P 439125-08-3P 439125-13-0P 439291-36-8P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 1802-16-0P, 3-Pyridinepropanal 62656-49-9P, 3-Thiophenepropanal
92028-92-7P, 4-Quinolinebutanoic acid 120690-80-4P, 4-Pyridinepropanal
143353-85-9P 152235-55-7P 152235-56-8P 153893-09-5P,
1H-Benzimidazole-1-propanal 166947-15-5P 198557-85-6P 214694-76-5P
217977-02-1P 220721-98-2P 438045-97-7P 438045-98-8P 438045-99-9P
438046-00-5P 438046-01-6P 438046-02-7P 438046-03-8P 438046-04-9P
438046-05-0P 438046-06-1P 438046-08-3P 438046-09-4P 438046-10-7P
438046-11-8P 438046-13-0P 438046-14-1P 438046-16-3P 438046-17-4P
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439106-51-1P 439106-52-2P, 4-Quinolinepentanoic acid 439106-53-3P,
4-Quinolinepentanal 439106-54-4P 439106-55-5P 439106-56-6P
439106-57-7P 439106-58-8P 439106-59-9P 439106-60-2P 439106-61-3P
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439106-91-9P 439106-92-0P 439106-93-1P 439106-95-3P 439106-96-4P
439106-97-5P 439106-98-6P, 1H-Pyrrolo[2,3-b]pyridine-1-propanal
439106-99-7P 439107-01-4P, 3H-Imidazo[4,5-c]pyridine-3-propanal
439107-02-5P, 1H-Imidazo[4,5-c]pyridine-1-propanal 439107-03-6P,
3H-Imidazo[4,5-b]pyridine-3-propanal 439107-04-7P 439107-05-8P
439107-06-9P 439107-07-0P 439107-08-1P 439107-09-2P 439107-10-5P
439107-12-7P, 3-Quinolinepropanal 439107-13-8P 439107-14-9P
439107-15-0P 439107-16-1P 439107-17-2P 439107-18-3P 439107-24-1P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial

infections)

IT 438046-12-9P 438046-19-6P 438046-22-1P 438046-24-3P 438046-26-5P
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439099-75-9P 439099-77-1P 439099-90-8P 439100-01-3P 439100-05-7P
439100-10-4P 439100-25-1P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 50-66-8 51-17-2, Benzimidazole 54-16-0, reactions 55-22-1,
4-Pyridinecarboxylic acid, reactions 59-00-7 59-67-6,
3-Pyridinecarboxylic acid, reactions 68-95-1 79-91-4 83-10-3
87-51-4, 1H-Indole-3-acetic acid, reactions 88-14-2, 2-Furancarboxylic acid 93-10-7, 2-Quinolinecarboxylic acid 96-32-2, Methyl bromoacetate
96-34-4 98-79-3 98-97-5, Pyrazinecarboxylic acid 98-98-6,
2-Pyridinecarboxylic acid 100-28-7 102-36-3 103-71-9,
Isocyanatobenzene, reactions 104-12-1 104-53-0, 3-Phenyl propionaldehyde 104-98-3 107-02-8, Acrylaldehyde, reactions
133-32-4, 1H-Indole-3-butanoic acid 156-06-9 271-63-6,
1H-Pyrrolo[2,3-b]pyridine 272-97-9, 1H-Imidazo[4,5-c]pyridine
273-21-2, 1H-Imidazo[4,5-b]pyridine 329-01-1 389-08-2 392-12-1
402-61-9 443-73-2 475-11-6 486-74-8, 4-Quinolinecarboxylic acid
488-93-7, 3-Furancarboxylic acid 496-41-3, 2-Benzofurancarboxylic acid
499-04-7 500-05-0 501-81-5, 3-Pyridineacetic acid 532-55-8, Benzoyl isothiocyanate 532-91-2 541-88-8, Chloroacetic anhydride 583-08-4
585-68-2 609-71-2 611-73-4 622-78-6 623-51-8 634-97-9,
1H-Pyrrole-2-carboxylic acid 645-12-5 645-65-8, 1H-Imidazole-4-acetic acid 670-95-1 700-87-8 769-52-8 771-81-3 779-27-1 824-40-8
830-96-6, 1H-Indole-3-propanoic acid 874-24-8 935-13-7,
2-Furanpropanoic acid 1013-88-3 1074-59-5, 1H-Imidazole-4-propanoic acid 1074-89-1 1126-74-5 1131-09-5, Benzo[b]thiophene-3-acetic acid
1136-45-4 1136-87-4 1136-88-5 1195-45-5 1196-57-2,
2(1H)-Quinoxalinone 1204-06-4 1218-34-4 1467-70-5 1477-49-2
1477-50-5, 1H-Indole-2-carboxylic acid 1618-34-4 1632-84-4 1912-43-2
1912-48-7 1918-77-0, 2-Thiopheneacetic acid 1943-82-4 2131-61-5
2131-64-8 2164-65-0 2257-09-2 2373-80-0 2386-28-9 2398-81-4
2510-36-3 2635-75-8, Benzo[b]thiophene-4-acetic acid 2637-37-8,
2(1H)-Quinolinethione 2745-26-8, 2-Furanacetic acid 2815-95-4,
1,3-Benzodioxole-5-propanoic acid 2859-67-8, 3-Pyridinepropanol
2861-28-1, 1,3-Benzodioxole-5-acetic acid 2882-15-7 2909-38-8
2942-59-8 3153-37-5, Methyl 4-Chlorobutanoate 3167-49-5 3173-56-6
3222-47-7 3222-56-8 3265-58-5 3288-04-8 3320-83-0 3320-86-3
3320-87-4 3395-91-3, Methyl 3-Bromopropanoate 3405-77-4 3460-49-9
3465-72-3 3471-31-6 3663-80-7 3694-57-3 3724-19-4,
3-Pyridinepropanoic acid 4009-98-7 4075-59-6 4100-13-4,
1,2,3-Thiadiazole-4-carboxylic acid 4192-31-8 4302-66-3 4363-93-3,
4-Quinolinecarboxaldehyde 4382-54-1 4412-96-8 4461-33-0, Benzoyl isocyanate 4572-80-9 4635-59-0, 4-Chlorobutyryl chloride 4650-60-6
4653-08-1 4653-11-6, 2-Thiophenebutanoic acid 4940-39-0 5006-45-1
5006-66-6 5241-64-5 5326-89-6 5333-34-6 5334-40-7 5345-47-1
5354-94-9 5395-71-1 5399-21-3 5416-93-3 5424-01-1 5438-71-1
5439-51-0 5454-83-1, Methyl 5-bromopentanoate 5461-32-5 5470-96-2,
2-Quinolinecarboxaldehyde 5521-55-1 5657-19-2 5678-07-9 5733-86-8
5744-59-2 5928-51-8, 2-Thiophenepropanoic acid 5952-92-1 6480-68-8,
3-Quinoline carboxylic acid. 6625-08-7 6947-94-0 6962-54-5,
2(1H)-Quinoxalinethione 6964-21-2, 3-Thiopheneacetic acid 6973-60-0
7028-67-3 7152-24-1 7164-43-4 7252-83-7 7340-22-9 7384-17-0
7394-79-8 7579-20-6, 3-Amino isonicotinic acid 7675-01-6 10002-29-6
10128-71-9 10231-46-6 10242-15-6 10351-19-6 13115-43-0,
2-Pyridineacetic acid 13139-14-5 13471-68-6 13471-69-7 13610-49-6
13610-59-8 13669-42-6, 3-Quinolinecarboxaldehyde 14617-13-1
14939-93-6 15268-31-2 15733-89-8 15863-41-9 16315-59-6
16413-26-6 16441-28-4 16498-81-0 16727-43-8 16730-20-4
16874-33-2 17153-20-7 17288-40-3 17608-09-2 17608-10-5

17784-60-0 17874-79-2 17969-20-9 18212-21-0 18213-77-9
18559-42-7 18908-07-1 18967-42-5 18967-44-7 19752-09-1
19771-63-2 20905-98-0, 3-Thiophenepropanol 20924-05-4 21169-71-1,
5-Isoxazolecarboxylic acid 21202-42-6 21714-25-0 21801-79-6
21905-86-2, 4-Cinnolinecarboxylic acid 22876-16-0 23118-26-5
23138-64-9 23165-60-8 23165-64-2 23249-97-0, 1H-Benzimidazole-2-
propanoic acid 23353-14-2 23695-15-0 23814-12-2,
1H-Benzotriazole-5-carboxylic acid 23945-44-0 24032-84-6 24195-07-1
24786-75-2 25503-90-6 25947-11-9 26030-46-6 26976-83-0
27006-82-2 27283-98-3 27372-38-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 27693-49-8 28162-63-2 28395-76-8 28479-19-8 28648-87-5
29198-86-5, 2-Benzothiazolepropanoic acid 29544-08-9 29711-79-3
29953-71-7 30113-83-8 30149-93-0 30280-44-5 30529-70-5
30994-18-4 31090-12-7 31909-01-0, Benzo[b]thiophene-2-butanoic acid
32084-55-2 32459-62-4 32998-25-7 33484-67-2 33955-17-8
34014-51-2 35037-73-1 35620-71-4 35794-78-6 37527-66-5
37718-11-9, 1H-Pyrazole-4-carboxylic acid 38980-93-7 39091-01-5
39116-31-9 40397-95-3 40397-96-4 40432-84-6 40465-45-0
40511-41-9 40532-06-7 41303-44-0, 1,3-Benzodioxole-5-butanoic acid
41680-34-6 41827-12-7 42046-56-0 42346-68-9 42831-50-5
46118-95-0 49647-20-3 50479-11-3 50528-53-5 50654-94-9
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53137-27-2 54132-76-2 54367-66-7 54557-81-2 55335-06-3
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57338-76-8 57910-98-2 58417-15-5 58749-51-2 59377-19-4
59377-20-7 59741-04-7 59776-60-2 61070-20-0 61070-22-2
63224-35-1 63429-99-2 64700-15-8 65101-82-8 65303-82-4
65476-24-6 65489-71-6 66158-33-6 67367-37-7 67406-38-6
67752-29-8, 4-Quinolinepropanoic acid 68622-14-0 69001-90-7
69922-28-7 70165-31-0 70984-52-0 71089-42-4 71239-85-5
71953-90-7 74458-92-7 74470-23-8 75239-13-3 76641-47-9
77628-51-4 78875-63-5 79720-70-0 80866-93-9 81103-11-9
81124-50-7 81124-51-8 83297-18-1 84030-19-3 84228-93-3
84370-87-6 84381-54-4 84891-19-0 86317-36-4 86608-70-0
87364-84-9 87392-05-0 87873-72-1 88768-45-0 89364-31-8
89711-08-0 91092-95-4 94192-18-4 94671-25-7 95444-36-3
98169-56-3 98266-33-2 99185-87-2 100068-17-5 101736-22-5
103987-16-2 103989-10-2 104612-36-4 106833-09-4 107367-98-6
107755-96-4 113100-53-1 113405-11-1, 4-Benzofuranacetic acid
113594-93-7 115311-44-9 116578-59-7 116611-64-4 117162-85-3
117724-63-7 119434-75-2 119923-27-2 120118-99-2 121996-14-3
123617-80-1, 3-Furanacetic acid 127926-81-2 128455-63-0 128625-52-5,
PyBOP 131825-41-7 132740-43-3 134107-69-0 135111-48-7
135264-38-9 137726-00-2 138775-06-1 139768-71-1 143353-82-6
144060-98-0 158063-66-2 159178-03-7 166196-73-2 169213-78-9
169555-95-7 174523-99-0, 3-Quinolinepropanol 175136-92-2 175136-93-3
175137-58-3 175201-51-1 175201-69-1 175201-94-2 176446-74-5
182500-26-1 183302-68-3 185300-51-0 186589-03-7 187028-77-9
190774-55-1 190774-56-2 195447-81-5 197585-42-5 198069-08-8
198348-89-9 198482-51-8 200816-06-4 202599-29-9 205528-30-9
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245322-47-8 246022-34-4 254880-57-4 254983-57-8 255874-79-4
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263160-43-6 263904-51-4 272437-91-9 276880-59-2 280133-38-2
280140-69-4 281232-20-0 286436-20-2 286832-96-0 301177-23-1
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338394-79-9 338408-38-1 338408-48-3 338418-26-1 338753-06-3
338778-85-1 338959-80-1 339011-93-7
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT 339012-78-1 339018-24-5 339030-37-4 339030-73-8 339276-36-7
343373-12-6 353245-98-4 386715-41-9 387350-60-9 387350-63-2
439106-30-6 439106-49-7 439106-66-8 439106-68-0 439106-73-7
439106-75-9 439106-79-3 439106-81-7 439106-87-3 439106-90-8
439106-94-2 439107-00-3 439107-11-6 439107-35-4 439107-37-6
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439107-79-6 439107-86-5 439107-99-0 439108-04-0 439108-10-8
439108-12-0 439108-15-3 439108-20-0, 2-Pyrimidinepropanoic acid
439108-23-3 439108-42-6 439108-48-2 439108-79-9 439108-85-7
439109-09-8 439109-76-9 439109-77-0 439109-78-1 439109-80-5
439109-81-6 439109-82-7 439109-83-8 439125-01-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Jean-Francois, C; US 5747467 A 1998 HCAPLUS
(2) Pfizer Prod Inc; EP 1114826 A 2001 HCAPLUS
(3) Roussel, U; FR 2732684 A 1996 HCAPLUS
(4) Sugimoto, T; WO 9921869 A 1999 HCAPLUS
(5) Sugimoto, T; WO 9921870 A 1999 HCAPLUS
(6) Thomas, M; WO 0044761 A 2000 HCAPLUS

IT **439102-08-6P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

RN 439102-08-6 HCAPLUS

CN 6-Pteridinepropanamide, N-[(3aS,4R,6R,8R,9R,10R,12R,15R,15aS)-15-ethyltetradecahydro-8-methoxy-4,6,8,10,12,15a-hexamethyl-2,5,11,13-tetraoxo-9-[[3,4,6-trideoxy-3-(dimethylamino)-β-D-xylo-hexopyranosyl]oxy]-2H-furo[2,3-c]oxacyclotetradecin-3-yl]-1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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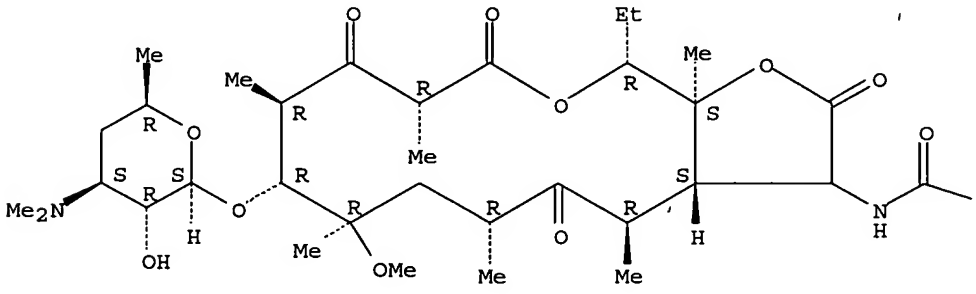

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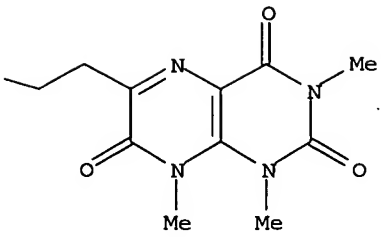
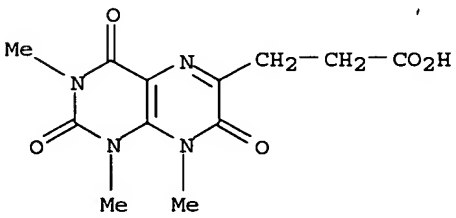
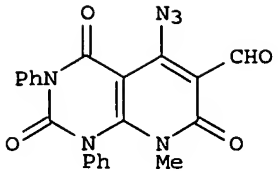


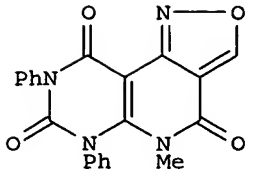
IT **76641-47-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)
RN 76641-47-9 HCAPLUS
CN 6-Pteridinepropanoic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)



L59 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:305021 HCAPLUS
DN 127:5057
ED Entered STN: 14 May 1997
TI Organic azides in heterocyclic synthesis. Part 22. Ring closure reactions of heterocyclic azides with the assistance of DSC
AU Dang Van Tinh; Stadlbauer, Wolfgang
CS Organic Synthesis Group, Institute of Organic Chemistry, Karl Franzens University of Graz, Austria
SO Molecules [Electronic Publication] (1996), 1, 201-206
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://science.springer.de/molec/bibs/1996/6010201.htm
PB Molecular Diversity Preservation International
DT Journal; (online computer file)
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 127:5057
GI



I



II

AB 5-Azidopyrido[2,3-d]pyrimidine-2,4,7-triones, e.g., I, or 6-azidouracils with reactive ortho substituents, such as aryl, acyl, or nitro, were prepared from the corresponding hydroxy compds. by chlorination (or tosylation) and reaction with sodium azide. The azides cyclized thermally to the corresponding indoles, isoxazoles, or furoxans, e.g., I → II. The cyclization conditions depended on the ortho substituents; the temperature ranged between 50 and 150°. Determination of the reaction temperature and suitable solvents was carried out with the aid of DSC. Also, reactions such as deoxygenation of the furoxans could be investigated by DSC in order to find suitable reaction conditions.

ST pyridopyrimidinetrione azido deriv prepn cyclization; uracil azido deriv prepn cyclization; cyclization azidopyridopyrimidinetrione azidouracil; indole fused derivs prepn; isoxazole fused derivs prepn; furoxan fused derivs prepn

IT Azides
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(heterocyclic; ring closure reactions studied by DSC)

IT Cyclization
(of heterocyclic azides studied by DSC)

IT Differential scanning calorimetry
(ring closure reactions of heterocyclic azides studied by DSC)

IT 42963-36-0 177082-44-9 177082-45-0 **177082-56-3** 189998-41-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure reactions of heterocyclic azides studied by DSC)

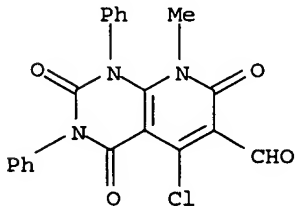
IT **189998-29-6P** 189998-34-3P 189998-36-5P 189998-38-7P 189998-46-7P 189998-48-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ring closure reactions of heterocyclic azides studied by DSC)

IT 33070-47-2P 189998-31-0P 189998-40-1P 189998-42-3P 189998-50-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring closure reactions of heterocyclic azides studied by DSC)

IT **177082-56-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure reactions of heterocyclic azides studied by DSC)

RN 177082-56-3 HCAPLUS

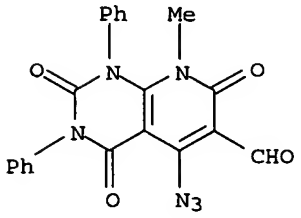
CN Pyrido[2,3-d]pyrimidine-6-carboxaldehyde, 5-chloro-1,2,3,4,7,8-hexahydro-8-methyl-2,4,7-trioxo-1,3-diphenyl- (9CI) (CA INDEX NAME)



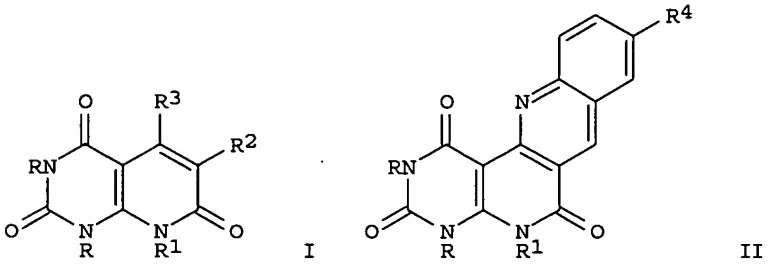
IT **189998-29-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ring closure reactions of heterocyclic azides studied by DSC)

Search done by Noble Jarrell

RN 189998-29-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxaldehyde, 5-azido-1,2,3,4,7,8-hexahydro-8-methyl-2,4,7-trioxo-1,3-diphenyl- (9CI) (CA INDEX NAME)



L59 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:147520 HCAPLUS
DN 125:10732
ED Entered STN: 13 Mar 1996
TI Ring closure reaction of 5-hydroxypyrido[2,3-d]pyrimidine-2,4,7-triones to benzo[b]pyrimido[4,5-h]1,6-naphthyridine-1,3,6-triones
AU Khattab, Ahmed F. A.; Dang Van Tinh; Stadlbauer, Wolfgang
CS Chem. Dep., Fac. Sci., Menoufeia, Egypt
SO Journal fuer Praktische Chemie/Chemiker-Zeitung (1996), 338(2), 151-6
CODEN: JPCCEM; ISSN: 0941-1216
PB Barth
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
GI



I II

AB N-substituted aminouracils reacted with malonates by cyclocondensation to pyridopyrimidinetriones I (R, R1 = Me, Ph; R2 = H, Ph, CH2Ph; R3 = OH). The condensation of I (R = R1 = Me; R2 = H) with CH(OEt)3 and aniline gave the corresponding 6-phenylaminomethylene compound Halogenation of I (R1 = Me) with POCl3 led to 5,7-dichloro compds. by cleavage of the Me-group at N-8. The Vilsmeier reaction of I afforded chloroformyl derivs. I (R2 = CHO; R3 = Cl), which cyclized with arylamines to give benzopyrimidonaphthyridinetriones II (R4 = H, Me, Cl, F, NO2). II were obtained independently by reaction of I (R3 = OTs, Ts = tosyl) with arylamines via the corresponding 5-arylamino compds. and subsequent Vilsmeier formylation.
ST benzopyrimidonaphthyridine prepn; aminouracil malonate cyclocondensation; pyridopyrimidine prepn Vilsmeier formylation
IT Cyclocondensation reaction
(preparation of benzopyrimidonaphthyridinetriones by cyclization of hydroxypyridopyrimidinetriones)
IT 62-53-3, Aniline, reactions 83-13-6, Diethyl 2-phenylmalonate
100-01-6, 4-Nitroaniline, reactions 105-53-3, Diethyl malonate
106-47-8, 4-Chloroaniline, reactions 106-49-0, 4-Methylaniline,

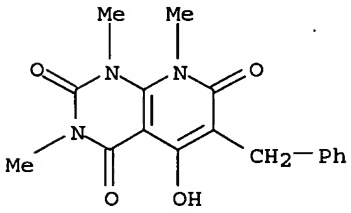
reactions 371-40-4, 4-Fluoroaniline 607-81-8, Diethyl benzylmalonate 5770-42-3 7278-51-5 66400-26-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzopyrimidonaphthyridinetriones by cyclization of hydroxypyridopyrimidinetriones)

IT 93738-66-0P 137278-09-2P 177082-44-9P 177082-45-0P 177082-46-1P **177082-47-2P 177082-48-3P 177082-55-2P** **177082-56-3P 177082-57-4P** 177082-58-5P 177082-59-6P 177082-60-9P 177082-61-0P 177082-62-1P 177082-63-2P 177082-64-3P 177082-65-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzopyrimidonaphthyridinetriones by cyclization of hydroxypyridopyrimidinetriones)

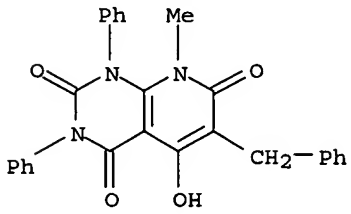
IT 137278-13-8P 177082-49-4P 177082-50-7P 177082-51-8P 177082-52-9P 177082-53-0P 177082-54-1P 177082-66-5P 177082-67-6P 177082-68-7P 177082-69-8P 177082-70-1P 177082-71-2P 177082-72-3P 177082-73-4P 177082-74-5P 177082-75-6P 177082-76-7P 177082-77-8P 177082-78-9P 177082-79-0P 177082-80-3P 177082-81-4P 177082-82-5P 177082-83-6P 177082-84-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzopyrimidonaphthyridinetriones by cyclization of hydroxypyridopyrimidinetriones)

IT **177082-47-2P 177082-48-3P 177082-55-2P** **177082-56-3P 177082-57-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzopyrimidonaphthyridinetriones by cyclization of hydroxypyridopyrimidinetriones)

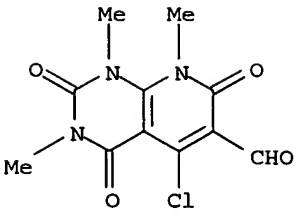
RN 177082-47-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,8-trimethyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



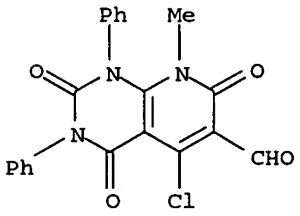
RN 177082-48-3 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-8-methyl-1,3-diphenyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



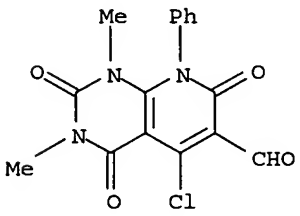
RN 177082-55-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxaldehyde, 5-chloro-1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)



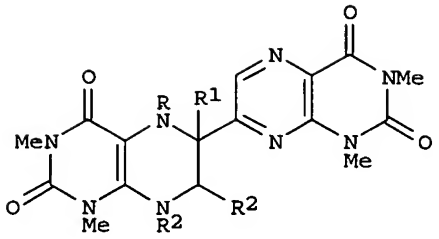
RN 177082-56-3 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxaldehyde, 5-chloro-1,2,3,4,7,8-hexahydro-8-methyl-2,4,7-trioxo-1,3-diphenyl- (9CI) (CA INDEX NAME)



RN 177082-57-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxaldehyde, 5-chloro-1,2,3,4,7,8-hexahydro-1,3-dimethyl-2,4,7-trioxo-8-phenyl- (9CI) (CA INDEX NAME)



L59 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:394467 HCAPLUS
DN 122:214436
ED Entered STN: 04 Mar 1995
TI Pteridines CII. Synthesis and characterization of dimeric lumazines
AU Koul, Ashok; Wagner, Thomas; Pfleiderer, Wolfgang
CS Fakultaet Chemie, Univ. Konstanz, Konstanz, D-78434, Germany
SO Pteridines (1994), 5(4), 121-8
CODEN: PTRDEO; ISSN: 0933-4807
PB International Society of Pteridinology
DT Journal
LA English
CC 33-9 (Carbohydrates)
GI



I

AB Reduction of 1,3-dimethyllumazine by zinc dust in Ac2O/AcOH leads to the formation of 6-7 connected bis-lumazinyl derivs. Depending on the reaction conditions either 7-(5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazin-6-yl)-1,3-dimethyllumazin I, (R = Ac, R1 = R2 = H) or isomeric 7-(5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazin-6-yl)-5-acetyl-5,6,7,8-tetrahydro-1,3-dimethyllumazines (II) are formed. Treatment of I (R = Ac, R1 = R2 = H) with MeOH/HCl gave I (R = R1 = R2 = H) which is oxidized by air to a very stable 7,8-dihydro derivative I (RR1 = bond, R2 = H) showing unexpected spectra properties. Further oxidation by KMnO4 afforded 6,7-bis-1,3-dimethyllumazinyl I (RR1 = bond, R22 = bond). Isomeric 6,6- and 7,7-bis-1,3-dimethyllumazinyls were also synthesized from 6-chloro- and 7-chloro-1,3-dimethyllumazine, resp., in a nickel catalyzed dimerization reaction. The various structures were proven by spectral means, elemental analyses and an x-ray anal. of II. Comparisons of the structural features are mainly based on UV data.

ST lumazine dimeric

IT 84689-47-4, 6-Chloro-1,3-dimethyllumazine 84689-48-5, 6-Bromo-1,3-dimethyllumazine 84689-49-6, 7-Chloro-1,3-dimethyllumazine 84689-50-9, 2,4(1H,3H)-Pteridinedione, 7-bromo-1,3-dimethyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dimeric lumazines)

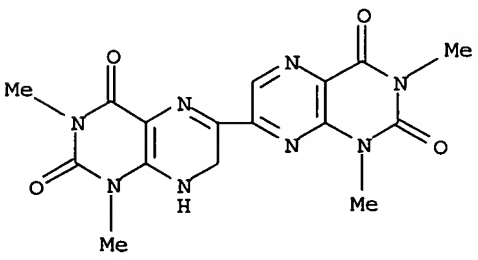
IT 13401-18-8P, 1,3-Dimethyllumazine 161959-61-1P 161959-62-2P **161959-63-3P** 161959-66-6P 161959-68-8P 161959-71-3P 161959-73-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dimeric lumazines)

IT 161959-60-0P 161959-64-4P 161959-65-5P 161959-67-7P 161959-69-9P 161959-70-2P 161959-72-4P 161959-74-6P 161959-75-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dimeric lumazines)

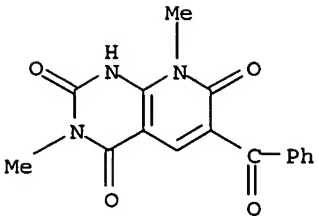
IT **161959-63-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dimeric lumazines)

RN 161959-63-3 HCAPLUS

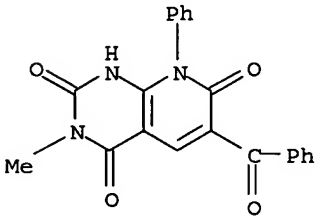
CN [6,7'-Bipteridine]-2,2',4,4'(1H,1'H,3H,3'H)-tetrone, 7,8-dihydro-1,1',3,3'-tetramethyl- (9CI) (CA INDEX NAME)



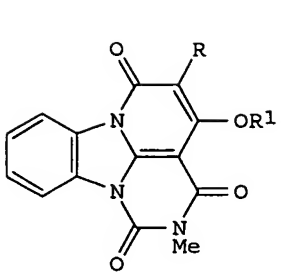
L59 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:491340 HCAPLUS
DN 119:91340
ED Entered STN: 04 Sep 1993
TI Inhibition of shikonin biosynthesis by photodegradation products of FMN
AU Tabata, Mamoru; Yazaki, Kazufumi; Nishikawa, Yumiko; Yoneda, Fumio
CS Fac. Pharm. Sci., Kyoto Univ., Kyoto, 606, Japan
SO Phytochemistry (1993), 32(6), 1439-42
CODEN: PYTCAS; ISSN: 0031-9422
DT Journal
LA English
CC 11-2 (Plant Biochemistry)
AB Shikonin biosynthesis in cell suspension cultures of Lithospermum erythrorhizon, which fails to occur under either white or blue light, was strongly inhibited by lumiflavin, a photodegrdn. product of FMN. A study on the structure-activity relation with 4 riboflavin analogs showed that the isoalloxazine moiety is essential for the inhibition of shikonin biosynthesis. These results, as well as the accumulation of biosynthetic precursors, p-hydroxybenzoic acid and its O-glucoside, in the cells irradiated with light, suggest that light would inactivate a flavoprotein necessary for an enzymic oxidation process leading to shikonin by decomposing the cofactor FMN into lumiflavin.
ST shikonin formation Lithospermum FMN; lumiflavin shikonin formation Lithospermum
IT Light
(shikonin formation by suspension cultures of Lithospermum erythrorhizon response to, FMN in relation to)
IT Lithospermum erythrorhizon
(shikonin formation by suspension cultures of, FMN photodegrdn. products effect on)
IT Molecular structure-biological activity relationship
(shikonin formation-inhibition, of riboflavin analogs, in Lithospermum erythrorhizon)
IT 517-89-5, Shikonin
RL: FORM (Formation, nonpreparative)
(formation of, by Lithospermum erythrorhizon suspension cultures, FMN photodegrdn. products effect on)
IT 99-96-7, p-Hydroxybenzoic acid, biological studies 10457-66-6, Geranylhydroquinone 15397-25-8 68631-48-1
RL: FORM (Formation, nonpreparative)
(formation of, by Lithospermum erythrorhizon suspension cultures, light effect on)
IT 1086-80-2, Lumichrome
RL: BIOL (Biological study)
(shikonin formation in Lithospermum erythrorhizon cell suspension cultures response to)
IT 92978-35-3 **92978-37-5** **92978-42-2** 93832-83-8
RL: BIOL (Biological study)
(shikonin formation in Lithospermum erythrorhizon response to, structure in relation to)
IT 146-17-8D, FMN, photodegrdn. products 1088-56-8, Lumiflavin
RL: BIOL (Biological study)
(shikonin formation inhibition by, in Lithospermum erythrorhizon suspension cultures)
IT **92978-37-5** **92978-42-2**
RL: BIOL (Biological study)
(shikonin formation in Lithospermum erythrorhizon response to, structure in relation to)
RN 92978-37-5 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3,8-dimethyl- (9CI) (CA INDEX NAME)



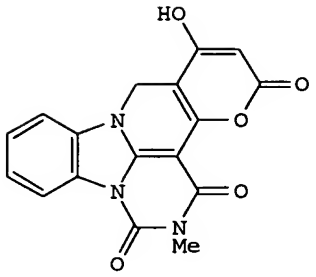
RN 92978-42-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3-methyl-8-phenyl- (9CI) (CA INDEX NAME)



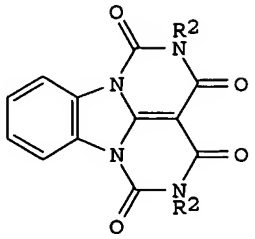
L59 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:559091 HCAPLUS
DN 115:159091
ED Entered STN: 18 Oct 1991
TI Benzimidazole condensed ring systems. 7. An entry to substituted 1H,6H-2,6a,10b-triazafluoranthene-1,3,6-(2H)-triones and related systems as possible chemotherapeutic agents
AU Badawey, El Sayed A. M.; Kappe, Thomas
CS Fac. Pharm., Univ. Alexandria, Egypt
SO Journal of Heterocyclic Chemistry (1991), 28(4), 995-8
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 10
OS CASREACT 115:159091
GI



I



II



III

AB The syntheses of some derivs. of three new benzimidazole condensed ring systems; namely, 1H,6H-2,6a,10b-triazafluoranthene-1,3,6(2H)-triones I (R = Me, Et, Bu, CH2Ph, Ph, R1 = H; R = R2 = Me, Bu; R = CH2Ph, R1 = Et; R = Ph, R1 = CONMe2), 1H,8H,11H-12-oxa-2,3a,7b-triazabenz[e]acephenanthrylene-1,3,8,11(2H)-tetrone II, and 1H,4H-2,5,6a,10b-tetrafluoroanthene-1,3,4,6(2H,5H)-tetrones III (R2 = H, Me) are described. I (R = Me, R1 = H; R = Ph, R1 = CONMe2) exhibited in vitro antibacterial activity. Four compds. were screened for in vitro anti-HIV activity and three compds. were evaluated for antileukemic potency but were inactive.

ST malonate cyclocondensation pyrimidobenzimidazoledione; methylbenzimidazole cyclocondensation ethoxycarbonyl isocyanate; fluoranthenethione triaza antibacterial; HIV inhibitor inactive triazafluoranthenetrione; leukemia neoplasm inhibitor inactive triazafluoranthenetrione; bactericide triazafluoranthenetrione; fluoranthenetetraone tetraaza inactive bactericide virucide; benzacephenanthrylenetetraone inactive bactericide virucide

IT Cyclocondensation reaction
(of malonates with pyrimidobenzimidazolediones, triazafluoranthenetriones from)

IT Bactericides, Disinfectants, and Antiseptics
(triazafluoranthenetrione derivs.)

IT Virus, animal
(human immunodeficiency, inhibitors, triazafluoroanthenetrione derivs. as inactive)

IT Neoplasm inhibitors
(leukemia, triazafluoranthenetrione derivs. as inactive)

IT 79-44-7, N,N-Dimethylcarbamoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with triazafluoranthenetrione derivative)

IT 615-15-6, 2-Methylbenzimidazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with ethoxycarbonyl isocyanate, tetraazafluoranthenetetrone from)

IT 19617-43-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with methylbenzimidazole, tetraazafluoranthenetetrone from)

IT 105-53-3, Diethyl malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrimidobenzimidazoledione, triazafluoranthenetrione derivative from)

IT 83-13-6, Diethyl phenylmalonate 133-08-4, Diethyl butylmalonate
133-13-1, Diethyl ethylmalonate 607-81-8, Diethyl benzylmalonate
609-08-5, Diethyl methylmalonate 15781-72-3, Bis-2,4,6-trichlorophenyl ethylmalonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrimidobenzimidazoledione, triazafluoranthenetrione from)

IT 94447-78-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with substituted malonates, triazafluoranthenetrione derivs. from)

IT **136296-10-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-HIV activity of)

IT **136296-08-7P 136296-09-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of)

IT **136296-03-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antileukemia activity of)

IT **136296-05-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ethylation of)

IT 136296-01-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 136296-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, antibacterial, and anti-HIV activity of)

IT 136296-07-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, antibacterial, anti-HIV, and antileukemia activity of)

IT **136296-04-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, butylation, and pharmacol. activity of)

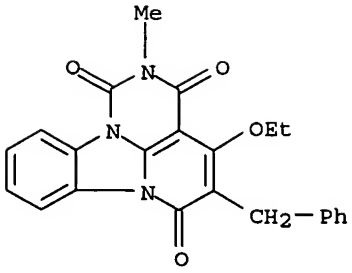
IT 136296-06-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, condensation of, with carbamoyl chloride, and antileukemia activity of)

IT **136296-02-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, methylation, and antibacterial activity of)

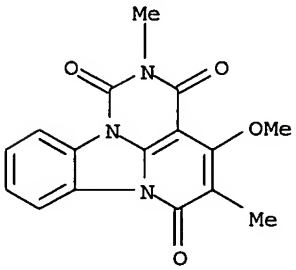
IT 136296-00-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, methylation, antibacterial, and anti-HIV activity of)

IT **136296-10-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-HIV activity of)

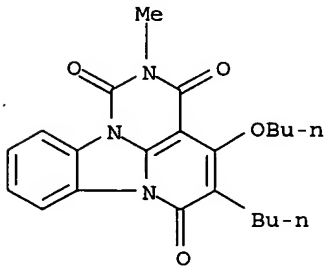
RN 136296-10-1 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 4-ethoxy-2-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



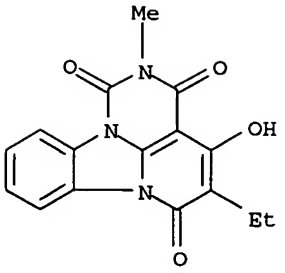
IT **136296-08-7P 136296-09-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of)
RN 136296-08-7 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)



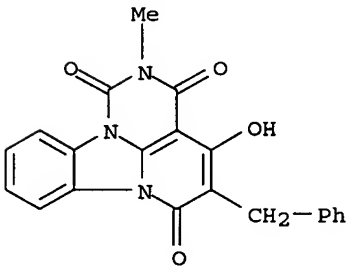
RN 136296-09-8 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 4-butoxy-5-butyl-2-methyl- (9CI) (CA INDEX NAME)



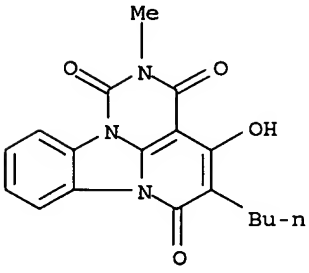
IT **136296-03-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antileukemia activity of)
RN 136296-03-2 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 5-ethyl-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



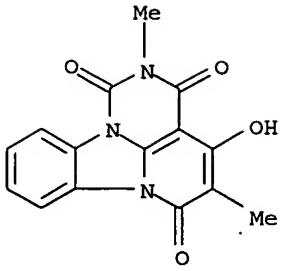
IT **136296-05-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ethylation of)
RN 136296-05-4 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 4-hydroxy-2-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



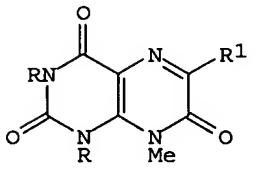
IT **136296-04-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, butylation, and pharmacol. activity of)
RN 136296-04-3 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 5-butyl-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



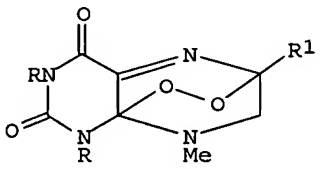
IT **136296-02-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, methylation, and antibacterial activity of)
RN 136296-02-1 HCAPLUS
CN 1H,6H-2,6a,10b-Triazafluoranthene-1,3,6(2H)-trione, 4-hydroxy-2,5-dimethyl- (9CI) (CA INDEX NAME)



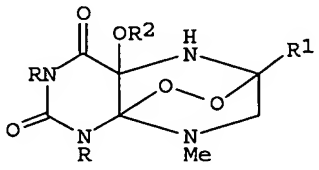
L59 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:428965 HCAPLUS
DN 115:28965
ED Entered STN: 27 Jul 1991
TI Photooxygenation of pteridine-2,4,7-triones
AU Nishio, Takehiko; Nishiyama, Tadashi; Omote, Yoshimori
CS Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Tetrahedron (1991), 47(18-19), 2979-90
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
CC 26-9 (Biomolecules and Their Synthetic Analogs)
OS CASREACT 115:28965
GI



I



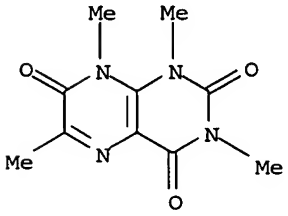
II



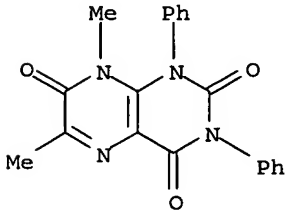
III

AB The pteridine-2,4,7-triones I (R, R1 = Me, Ph) reacted smoothly with singlet O to yield the 6,8'-endoperoxides II and III (R2 = H, Me, Et). On warming, II (R = Me, R1 = Ph) reverted to the starting pteridine-2,4,7-trione with liberation of singlet O which was confirmed by trapping expts. using typical singlet O acceptors.
ST pteridinetrione photoxygenation singlet oxygen; endoperoxide pteridinetrione; phenyltrimethylpteridinetrione endoperoxide prepn thermolysis
IT Oxidation, photochemical
(of pteridinetriones with singlet oxygen)
IT 134521-67-8P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and solvolysis of)
IT 7782-44-7, Oxygen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(photoxygenation by, of pteridinetriones)
IT **99069-70-2** 109853-23-8 **113088-54-3** 113088-55-4
RL: RCT (Reactant); RACT (Reactant or reagent)

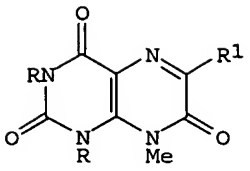
(photoxygenation of, with singlet oxygen)
IT 109853-25-0P 134521-64-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photolysis of)
IT 109853-24-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermolysis of, singlet oxygen from)
IT 134521-61-2P 134521-62-3P 134521-63-4P 134521-65-6P 134521-66-7P
134521-68-9P 134521-69-0P 134521-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 7782-44-7P, Oxygen, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(singlet, preparation of, by thermolysis of pteridinetrione endoperoxide)
IT **99069-70-2 113088-54-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photoxygenation of, with singlet oxygen)
RN 99069-70-2 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl- (6CI, 9CI) (CA INDEX NAME)



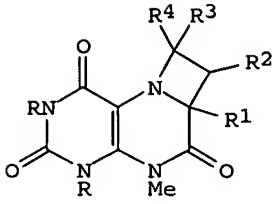
RN 113088-54-3 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 6,8-dimethyl-1,3-diphenyl- (9CI) (CA INDEX NAME)



L59 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:221670 HCAPLUS
DN 108:221670
ED Entered STN: 24 Jun 1988
TI Photochemical [2+s2] cycloadditions of the C = N bond of pteridine-2,4,7-triones to alkenes
AU Nishio, Takehiko; Nishiyama, Tadashi; Omote, Yoshimori
CS Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Liebigs Annalen der Chemie (1988), (5), 441-3
CODEN: LACHDL; ISSN: 0170-2041
DT Journal
LA English
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 108:221670
GI



I



II

AB Irradiation of pteridine-2,4,7-triones I (R = Me, Ph; R1 = Me) in the presence of electron-deficient and neutral alkenes, R2CH:CR3R4 (R2 = H, cyano, Ph, CO2Me; R3 = H, Me, Ph; R4 = cyano, CO2Me, Ph) gave azetidines II via [2 + 2] cycloaddn. reaction of the C=N double bond of I to the alkenes in a regiospecific manner. Irradiation of I (R = Me, Ph; R1 = Ph) did not give photocycloadduct with methacrylonitrile.

ST pteridinetrione alkene cycloaddn photochem regiochem

IT Regiochemistry
(of photochem. cycloaddn. of pteridinetriones to electron-deficient alkenes)

IT Cycloaddition reaction
([2+2], photochem., of pteridinetriones to electron-deficient alkenes, azetidines from)

IT 109-92-2, Ethyl vinyl ether 110-83-8, Cyclohexene, reactions 115-11-7, Isobutene, reactions 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted photochem. cycloaddn. of, with pteridinetriones)

IT 80-62-6, Methyl methacrylate 107-13-1, Acrylonitrile, reactions 126-98-7, Methacrylonitrile 530-48-3, 1,1-Diphenylethylene 624-49-7, Dimethyl fumarate 764-42-1, Fumaronitrile 4360-47-8, Cinnamonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn. of, with pteridinetriones)

IT 109853-23-8P 113088-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and attempted photochem. cycloaddn. of, with methacrylonitrile)

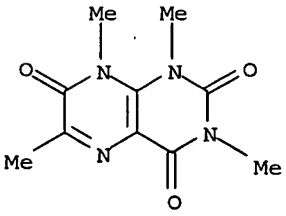
IT **99069-70-2P 113088-54-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cycloaddn. of, azetidines from)

IT 113088-56-5P 113088-57-6P 113088-58-7P 113088-59-8P 113088-60-1P 113088-61-2P 113088-62-3P 113088-63-4P 113088-64-5P 113088-65-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **99069-70-2P 113088-54-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cycloaddn. of, azetidines from)

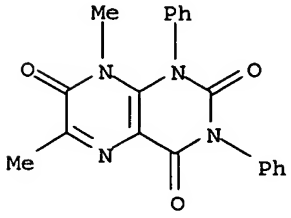
RN 99069-70-2 HCAPLUS

CN 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl- (6CI, 9CI) (CA INDEX NAME)

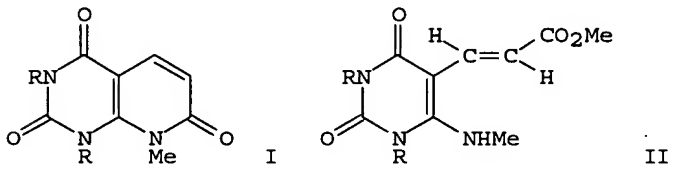


RN 113088-54-3 HCAPLUS

CN 2,4,7(1H,3H,8H)-Pteridinetrione, 6,8-dimethyl-1,3-diphenyl- (9CI) (CA INDEX NAME)

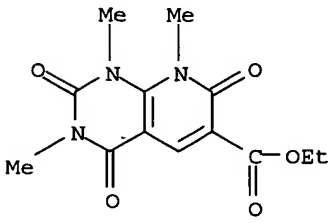


L59 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:112382 HCAPLUS
DN 108:112382
ED Entered STN: 01 Apr 1988
TI An improved synthesis of pyrido[2,3-d]pyrimidines
AU Ogura, Haruo; Mizuno, Yoshihisa; Kawahara, Norio
CS Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SO Journal of Heterocyclic Chemistry (1987), 24(5), 1453-5
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 26
OS CASREACT 108:112382
GI



AB 6-(Methylamino)uracils were heated with Me propiolate in CH2Cl2, and the reaction mixts. were irradiated in Me2CO to give pyridopyrimidines I (R = Me, Et). I were accompanied by addition products II.
ST pyridopyrimidinetrione; aminouracil cycloaddn cyclocondensation propiolate; photochem cycloaddn cyclocondensation aminouracil
IT Cyclocondensation reaction
(photochem. cycloaddn. and, of aminouracils with propiolate ester)
IT Cycloaddition reaction
(photochem. cyclocondensation and, of aminouracils with propiolate ester)
IT 87-13-8, Diethyl (ethoxymethylene)malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with aminouracil derivative)
IT 922-67-8, Methyl propiolate
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn.-cyclocondensation reaction of, with aminouracils)
IT 5770-42-3 101774-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn.-cyclocondensation reaction of, with propiolate ester)
IT 2672-58-4P, Trimethyl 1,3,5-benzenetricarboxylate 90402-67-8P
113306-24-4P 113306-25-5P 113306-26-6P 113306-27-7P
113306-28-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **113306-28-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 113306-28-8 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester (9CI) (CA INDEX NAME)



L59 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1984:611077 HCAPLUS
DN 101:211077
TI Synthesis and properties of 2,3,4,8-tetrahydro-2,4-dioxopyrido[2,3-d]pyrimidines (5-deazalumazines) and their bis-compounds
AU Nagamatsu, Tomohisa; Koga, Masakazu; Yoneda, Fumio
CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan
SO Chemical & Pharmaceutical Bulletin (1984), 32(5), 1699-708
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
GI For diagram(s), see printed CA Issue.
AB Et pyrido[2,3-d]pyrimidine-6-carboxylates I (R = Me, Et, octyl, Ph, 4-MeC6H4, 4-ClC6H4; R1 = Me, Ph and their bis-compds. II (n = 6, 8, 10, 12) were synthesized by condensation of methyluracils III with ClCR1:C(CHO)CO2Et. Hydrolysis of I and II with base resulted in a novel rearrangement of a substituent at the 7-position onto the 6-substituent to give the pyrido[2,3-d]pyrimidines IV and their bis-compds. V. The mechanism of the rearrangement was discussed.
ST oxopyridopyrimidines; deazalumazines; pyridopyrimidinecarboxylate dioxo hydrolysis rearrangement; alkylenebispyridopyrimidinecarboxylate hydrolysis rearrangement
IT Cyclocondensation reaction
(of aminomethyluracil with chloroformylpropenoates, deazalumazines from)
IT Rearrangement
(of deazalumazines, acylhexahydrotrioxopyridopyrimidines from)
IT 124-09-4, reactions 373-44-4 646-25-3 2783-17-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of chloromethyluracil)
IT 4318-56-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of)
IT 6642-31-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chloroformylphenylpropenoate)
IT 5759-63-7 5759-64-8 7269-95-6 58137-45-4 76896-60-1 83797-70-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chloroformylpropenoate derivative)
IT 85103-27-1 85103-28-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reactions of, with aminomethyluracils)
IT 92978-16-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of)

IT **92978-37-5P 92978-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with urea)

IT 87624-96-2P 87624-97-3P 87624-98-4P 87699-09-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with chloroformylcinnamate)

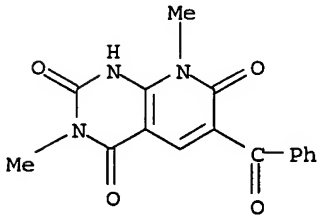
IT 92978-15-9P **92978-50-2P 92978-51-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 85103-13-5P 85103-14-6P 85103-20-4P 85103-21-5P 92978-27-3P
92978-28-4P 92978-29-5P 92978-30-8P 92978-31-9P 92978-32-0P
92978-33-1P 92978-34-2P 92978-35-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification-rearrangement of)

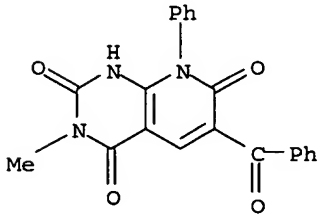
IT 85103-23-7P 85103-24-8P 85103-25-9P 85103-26-0P **92978-11-5P**
92978-12-6P 92978-13-7P 92978-14-8P
92978-17-1P 92978-18-2P 92978-19-3P 92978-20-6P 92978-21-7P
92978-22-8P 92978-23-9P 92978-24-0P 92978-25-1P **92978-36-4P**
92978-38-6P 92978-39-7P 92978-40-0P
92978-41-1P 92978-43-3P 92978-44-4P
92978-45-5P 92978-46-6P 92978-47-7P
92978-48-8P 92978-49-9P 92989-92-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **92978-37-5P 92978-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with urea)

RN 92978-37-5 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 92978-42-2 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3-methyl-8-phenyl- (9CI) (CA INDEX NAME)

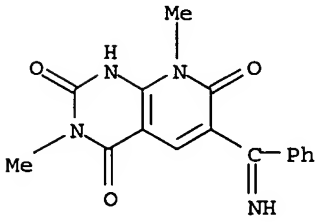


IT **92978-50-2P 92978-51-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

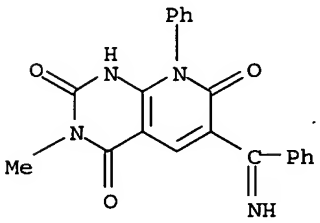
RN 92978-50-2 HCAPLUS

CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-(iminophenylmethyl)-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 92978-51-3 HCAPLUS

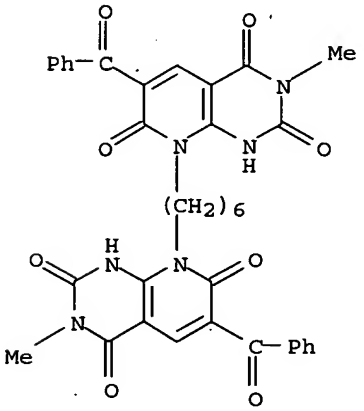
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-(iminophenylmethyl)-3-methyl-8-phenyl- (9CI) (CA INDEX NAME)



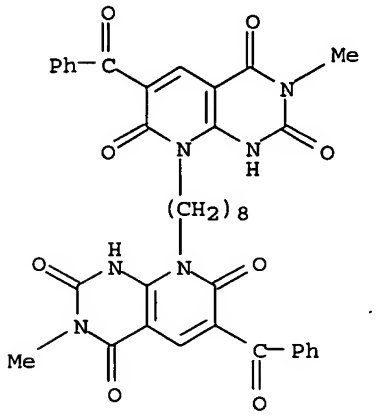
IT **92978-11-5P 92978-12-6P 92978-13-7P**
92978-14-8P 92978-36-4P 92978-38-6P
92978-39-7P 92978-40-0P 92978-41-1P
92978-43-3P 92978-44-4P 92978-45-5P
92978-46-6P 92978-47-7P 92978-48-8P
92978-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 92978-11-5 HCAPLUS

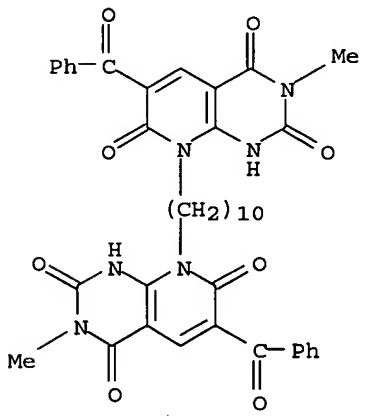
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 8,8'-(1,6-hexanediyl)bis[6-benzoyl-3-methyl- (9CI) (CA INDEX NAME)



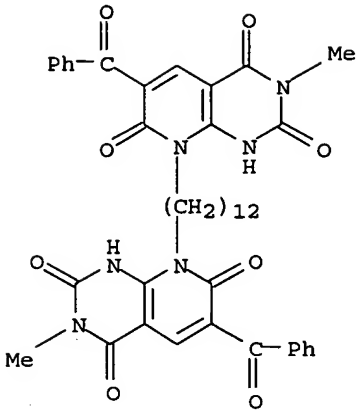
RN 92978-12-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 8,8'-(1,8-octanediyl)bis[6-benzoyl-3-methyl- (9CI) (CA INDEX NAME)



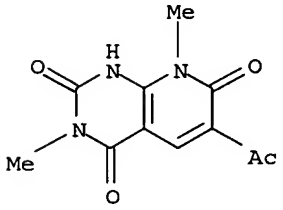
RN 92978-13-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 8,8'-(1,10-decanediyl)bis[6-benzoyl-3-methyl- (9CI) (CA INDEX NAME)



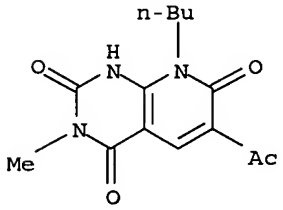
RN 92978-14-8 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 8,8'-(1,12-dodecanediyl)bis[6-benzoyl-3-methyl- (9CI) (CA INDEX NAME)



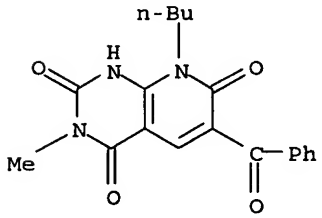
RN 92978-36-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-acetyl-3,8-dimethyl-
(9CI) (CA INDEX NAME)



RN 92978-38-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-acetyl-8-butyl-3-methyl-
(9CI) (CA INDEX NAME)

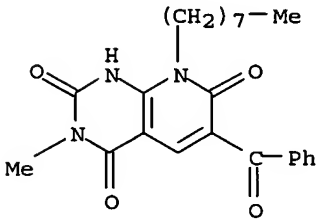


RN 92978-39-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-8-butyl-3-methyl-
(9CI) (CA INDEX NAME)

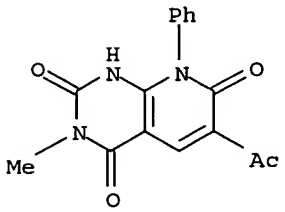


RN 92978-40-0 HCAPLUS

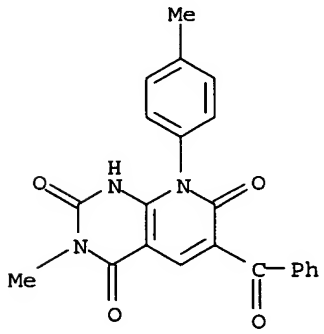
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3-methyl-8-octyl- (9CI) (CA INDEX NAME)



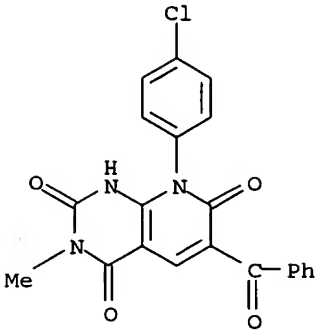
RN 92978-41-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-acetyl-3-methyl-8-phenyl- (9CI) (CA INDEX NAME)



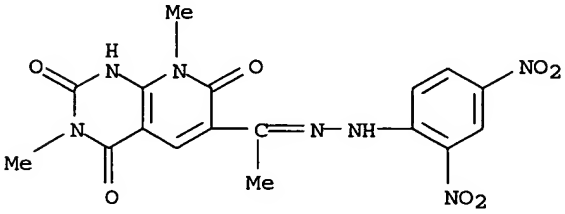
RN 92978-43-3 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-3-methyl-8-(4-methylphenyl)- (9CI) (CA INDEX NAME)



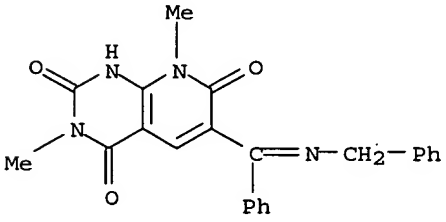
RN 92978-44-4 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-benzoyl-8-(4-chlorophenyl)-3-methyl- (9CI) (CA INDEX NAME)



RN 92978-45-5 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-[1-[(2,4-dinitrophenyl)hydrazono]ethyl]-3,8-dimethyl- (9CI) (CA INDEX NAME)

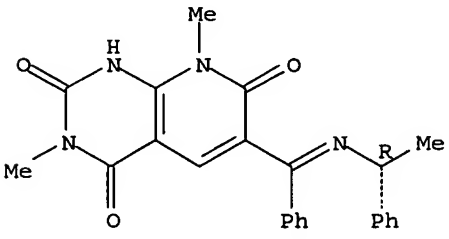


RN 92978-46-6 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 3,8-dimethyl-6-[phenyl[(phenylmethyl)imino]methyl]- (9CI) (CA INDEX NAME)



RN 92978-47-7 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 3,8-dimethyl-6-[phenyl[(1-phenylethyl)imino]methyl]-, (R)- (9CI) (CA INDEX NAME)

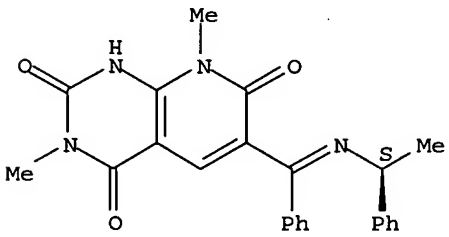
Absolute stereochemistry.
Double bond geometry unknown.



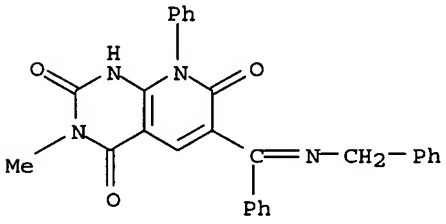
RN 92978-48-8 HCAPLUS

CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 3,8-dimethyl-6-[phenyl[(1-phenylethyl)imino]methyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 92978-49-9 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 3-methyl-8-phenyl-6-[phenyl[(phenylmethyl)imino]methyl]- (9CI) (CA INDEX NAME)



L59 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:197408 HCAPLUS
DN 98:197408
ED Entered STN: 12 May 1984
TI High- and low-potential flavin mimics (based on the pyrimidino[5,4-g]pteridine and imidazo[4,5-g]pteridine system). 1. General chemistry
AU Skibo, Edward B.; Bruice, Thomas C.
CS Dep. Chem., Univ. California, Santa Barbara, CA, 93106, USA
SO Journal of the American Chemical Society (1983), 105(10), 3304-15
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB I dissocs. to its anion (II) with a pKa of 1.18. Reduction of I (2 e-, 2 H+) gives III. Acid dissociation of the two pyrimido rings of III occurs simultaneously (pKa 5.51 and 5.56) to provide the dianion (IV). At pH 7.0, the two-electron reduction of II to IV is associated with an E0' of -0.346 V (NHE). This reduction potential is 148 mV more neg. than the corresponding reduction potential for a flavin. The II/IV couple is offered as a low-potential flavin mimic. Removal of the neg. charge of II by introduction of a Me group at N-1 provides V. The E0' for two-electron reduction of V is -0.127 V. The change in potential on comparing II and V is discussed. The kinetics and products formed in the hydrolysis of II and V are described. II is rather stable, hydrolyzing via HO- attack at the

10a-position to provide VI. Protonation of VI is associated with a pKa of 2.96. The solvolysis of V under anaerobic conditions also occurs by formation of a 10-hydroxyl adduct (VII), which undergoes ring opening to yield VIII. VII was characterized spectrally and VIII·K+ isolated. The pKa for dissociation of protonated VIII is 2.79. Under aerobic conditons VIII undergoes oxidative ring contraction and decarboxylation to provide IX, which undergoes an intramol. first-order rearrangement to yield X. VIII, when treated with strong base and then acidified, also undergoes a ring contraction in the absence of O2 to yield XI, which can be oxidized (nO2/Pt) to IX. The pKa for dissociation of XI is 8.5. Acid-catalyzed hydrolysis of V also yields XI. The E0' for two-electron reduction of IX to XI is +0.400 V vs. NHE. IX is suggested as a possible high-potential flavin mimic..

ST flavin mimic; pyrimidinopteridine flavin mimic; imidazopteridine flavin mimic

IT Flavins
RL: PRP (Properties)
(mimics, pyrimidino- and imidazopyridines)

IT Kinetics of hydrolysis
(of flavin mimics)

IT Electric potential
(reduction, of flavin mimics)

IT 82639-49-4 85282-74-2 85282-75-3 85282-76-4 85282-77-5 85282-78-6
RL: PRP (Properties)
(UV spectrum of)

IT 82639-46-1 82639-47-2 85282-68-4
RL: PRP (Properties)
(as flavin mimic)

IT 85282-64-0P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and ring cleavage of)

IT **85282-65-1P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and ring contraction and decarboxylation of)

IT 85282-70-8P
RL: PREP (Preparation)
(formation, ionization and oxidation of)

IT 82639-45-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(ionization and reduction of)

IT 82639-48-3 **85282-67-3**
RL: PROC (Process)
(ionization of)

IT **85282-63-9P** 85282-72-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ionization of)

IT **85282-62-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protonation of)

IT 2278-13-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with methylalloxan)

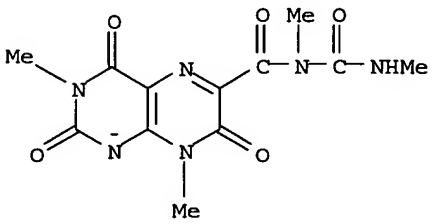
IT **85282-66-2P** 85282-69-5P 85282-71-9P 85282-73-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 82639-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reduction and solvolysis of)

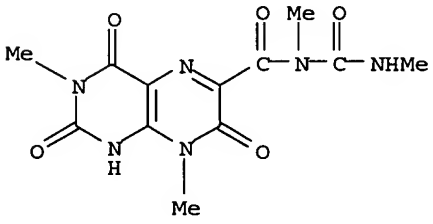
IT 61541-46-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylalloxan)

IT 5770-10-5
RL: RCT (Reactant); RACT (Reactant or reagent)

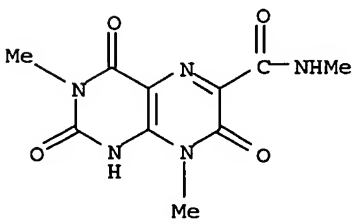
(reaction of, with methylbarbituric acid)
IT 2565-47-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitrosouracil derivative)
IT 2757-83-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with uracil amino derivs.)
IT 944-48-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT **85282-65-1P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and ring contraction and decarboxylation of)
RN 85282-65-1 HCAPLUS
CN 6-Pteridinecarboxamide, 1,2,3,4,7,8-hexahydro-N,3,8-trimethyl-N-[(methylamino)carbonyl]-2,4,7-trioxo-, ion(1-) (9CI) (CA INDEX NAME)



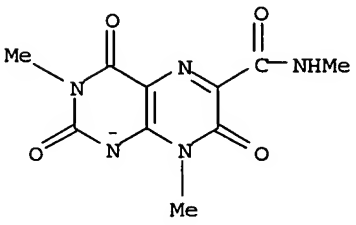
IT **85282-67-3**
RL: PROC (Process)
(ionization of)
RN 85282-67-3 HCAPLUS
CN 6-Pteridinecarboxamide, 1,2,3,4,7,8-hexahydro-N,3,8-trimethyl-N-[(methylamino)carbonyl]-2,4,7-trioxo- (9CI) (CA INDEX NAME)



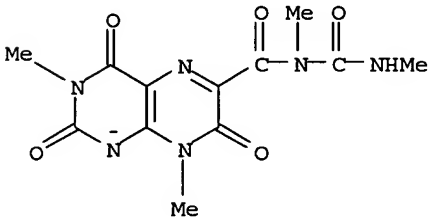
IT **85282-63-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ionization of)
RN 85282-63-9 HCAPLUS
CN 6-Pteridinecarboxamide, 1,2,3,4,7,8-hexahydro-N,3,8-trimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)



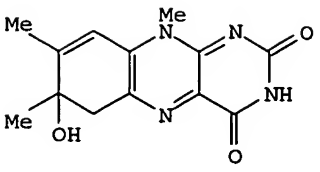
IT 85282-62-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protonation of)
RN 85282-62-8 HCAPLUS
CN 6-Pteridinecarboxamide, 1,2,3,4,7,8-hexahydro-N,3,8-trimethyl-2,4,7-trioxo-, ion(1-) (9CI) (CA INDEX NAME)



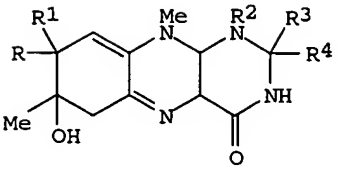
IT 85282-66-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85282-66-2 HCAPLUS
CN 6-Pteridinecarboxamide, 1,2,3,4,7,8-hexahydro-N,3,8-trimethyl-N-[(methylamino)carbonyl]-2,4,7-trioxo-, ion(1-), potassium (9CI) (CA INDEX NAME)



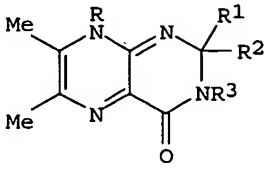
L59 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:496577 HCAPLUS
DN 95:96577
ED Entered STN: 12 May 1984
TI Chemiluminescence. III. The mechanism of the chemiluminescent autoxidation of 7-hydroxy-6,7-dihydrolumiflavin and some related pteridines
AU Addink, R.; Berends, W.
CS Biochem. Biophys. Lab., Univ. Technol., Delft, 2628 BC, Neth.
SO Tetrahedron (1981), 37(4), 833-41
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
CC 22-5 (Physical Organic Chemistry)
GI



I



II



III

AB In the conversion of the title flavin (I) to the 8-oxo compound II (RR1 = R3R4 = O, R2 = H) at pH >7, a nonoxidative and a subsequent oxidative phase were observed In the 1st phase, the formation of the intermediate II (R = Me, R1 = OH, R2 = H, R3R4 = O; RR1 = CH2, R2 = H, R3R4 = O; RR1 = CH2, R2 = H, R3 = R4 = OH) was established, and in the 2nd phase, the formation of the dioxetane II (RR1 = CH2O2, R2R3 = bond, R4 = O-) is postulated as the intermediate precursor in the light-giving step. The autoxidative chemiluminescence appeared to be a general feature of 8-substituted pteridines bearing a Me group at position 7, as the lumazines III (R = Me, R1R2 = O, R3 = H, Me) and the pterines III (R = Me, Et, CH2CH2OH, R1 = NH2, R2R3 = bond) gave similar intermediates. The chemiluminescence spectra and their quantum yields were determined

ST chemiluminescence autoxidn hydroxylumiflavin mechanism; flavin hydroxy chemiluminescence autoxidn mechanism; pteridine chemiluminescence autoxidn mechanism; lumiflavin hydroxy chemiluminescence autoxidn mechanism

IT Luminescence, chemi-
(in autoxidn. of hydroxydihydrolumiflavin, mechanism of)

IT Oxidation, aut-
(of hydroxydihydrolumiflavin, mechanism of chemiluminescent)

IT 3346-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of)

IT 5784-00-9 13045-86-8 13300-44-2 41964-37-8 78523-13-4 78523-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(chemiluminescent autoxidn. of, mechanism of)

IT 6743-25-5 **6743-26-6** 17813-28-4 25477-64-9 53301-40-9
RL: PRP (Properties)
(fluorescence spectrum of)

IT 78523-14-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)

IT 78523-09-8P 78523-10-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)

IT 78523-17-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV spectrum of)

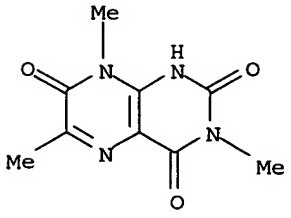
IT 78523-15-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence spectrum of)

IT 78523-11-2P 78523-12-3P 78523-17-8P 78535-42-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

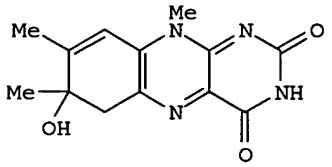
IT **6743-26-6**
RL: PRP (Properties)
(fluorescence spectrum of)

RN 6743-26-6 HCAPLUS

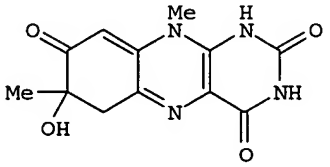
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)



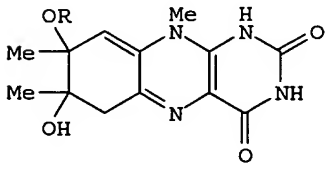
L59 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:479651 HCAPLUS
DN 95:79651
ED Entered STN: 12 May 1984
TI Chemiluminescence of a 6,7-dihydroflavin and some related pteridines
AU Addink, R.
CS Biochem. Biophys. Lab., Delft Univ. Technol., Delft, Neth.
SO Biolumin. Chemilumin., [Int. Symp. Anal. Appl. Biolumin. Chemilumin.], 2nd (1981), Meeting Date 1980, 507-14. Editor(s): DeLuca, Marlene A.; McElroy, William David. Publisher: Academic, New York, N. Y. CODEN: 45UJAC
DT Conference
LA English
CC 22-4 (Physical Organic Chemistry)
GI



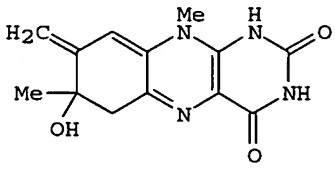
I



II



III



IV

AB Oxidation of 7-hydroxy-6,7-dihydrolumiflavine (I) in alkaline solns. gave the oxo compound II, accompanied by chemiluminescence. Under anaerobic conditions, treatment of I with base gave adducts III and IV (R = H, Me in each case). The chemiluminescence reaction involves formation of a dioxetane. The chemiluminescence autoxidn. of pteridine derivs. gave similar intermediates. The chemiluminescence autoxidn. of lumazine proceeds via a different mechanism.

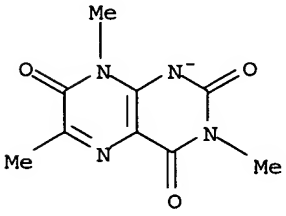
ST autoxidn dihydroflavin chemiluminescence; lumiflavine dihydro oxidn chemiluminescence; pteridine oxidn chemiluminescence

IT Luminescence, chemi-
(of hydroxydihydrolumiflavine and related pteridines under autoxidn. conditions)

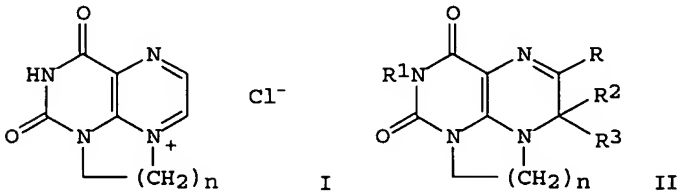
IT Oxidation, aut-
(of hydroxydihydrolumiflavine and related pteridines, chemiluminescence in)

IT 5784-00-9 13300-44-2
RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of, chemiluminescence from)
IT 53301-40-9P 78523-09-8P 78523-10-1P 78523-17-8P 78543-09-6P
78543-10-9P 78543-45-0P **78543-46-1P** 78543-47-2P
78543-48-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 41964-37-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with base under aerobic or anaerobic conditions, chemiluminescence from)
IT 1088-56-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with potassium tert-butoxide under aerobic conditions)
IT **78543-46-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78543-46-1 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl-, ion(1-) (9CI) (CA INDEX NAME)



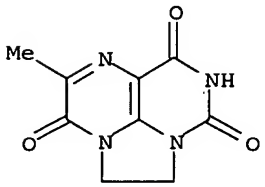
L59 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:175055 HCAPLUS
DN 94:175055
ED Entered STN: 12 May 1984
TI Pteridines. LXX. Synthesis and properties of 1,8-alkylene-bridged lumazines
AU Uhlmann, Eugen; Pfleiderer, Wolfgang
CS Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SO Heterocycles (1981), 15(1), 437-53
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22
GI



AB The lumazines I (n = 1, 2) and II (R = Me, R1 = H, R2R3 = CH2, n = 1, 2; R = R1 = Me, R2R3 = CH2, n = 1; R = R2 = Ph, R1 = H, R3 = OH, n = 1, 2) were prepared to determine the protonation site in lumazine. UV spectra indicate a mixture of ≥2 cationic species.
ST alkanolumazine prepn UV; UV alkanolumazine lumazine; protonation lumazine UV

IT Ultraviolet and visible spectra
(of alkanolumazines)
IT 2625-25-4 5774-32-3 7499-94-7 14892-98-9 19845-24-0 19845-25-1
35247-71-3 50256-19-4 50256-21-8 50256-22-9 51584-45-3
77178-60-0 77178-61-1 77178-62-2 77178-63-3 77178-64-4
77178-65-5 77178-66-6 77178-67-7 77178-68-8 77342-42-8
77358-24-8
RL: PRP (Properties)
(UV spectrum of)
IT 878-86-4 6630-30-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of)
IT 77178-38-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV spectra of)
IT 77178-44-0P 77178-45-1P 77178-46-2P 77178-50-8P
77178-54-2P 77178-55-3P 77178-57-5P 77178-58-6P 77178-59-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV spectrum of)
IT 66031-99-0P 66032-00-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and cyclization of)
IT 56075-69-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and nitrosation of)
IT 1320-51-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with cyanoacetate)
IT 77178-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with diacetyl)
IT 77178-51-9P 77178-53-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with glyoxal)
IT 17853-18-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with oxyalkanoates)
IT 77178-37-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with α-diketones)
IT 52850-69-8P 77178-36-0P 77178-47-3P 77178-48-4P 77178-49-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of)
IT 77178-41-7P 77178-42-8P 77178-52-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 17801-83-1P 77178-43-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation, cyclization, and UV spectrum of)
IT 77178-39-3P 77178-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation, mesylation, and UV spectra of)
IT 600-22-6 611-73-4 49653-17-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amino(hydroxyethylamino)uracil)
IT 156-87-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloronitrouracil)
IT 107-22-2 134-81-6 431-03-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diamino(hydroxyethyl)uracil)
IT 556-89-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethanolamine)
IT 105-56-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxyethylurea)
IT 141-43-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitrourea)
IT **77178-45-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV spectrum of)
RN 77178-45-1 HCAPLUS
CN 3H,8H-Imidazo[1,2,3-ij]pteridine-3,8,10(9H)-trione, 5,6-dihydro-2-methyl-(9CI) (CA INDEX NAME)



L59 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:103196 HCAPLUS
DN 94:103196
ED Entered STN: 12 May 1984
TI Specific enzyme inhibitors in vitamin biosynthesis. Part 3. The synthesis and inhibitory properties of some substrates and transition state analogs of riboflavin synthase
AU Al-Hassan, Saieba S.; Kulick, Russell J.; Livingstone, Daniel B.; Suckling, Colin J.; Wood, Hamish C. S.; Wrigglesworth, Roger; Ferone, Robert
CS Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, G1 1XL, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (12), 2645-56
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 7, 33
AB The tolerance of riboflavin synthase to bulky substituents was investigated by preparation of several substrate analogs. Lumazines and pyrido[2,3-d]-pyrimidines were prepared by condensation of α-diketones and β-keto-aldehydes resp. with amino-substituted uracils. Potential transition-state analogs, including 7-oxolumazines, 7-oxopyrido[2,3-d]pyrimidines, and 6,7-dioxolumazines were prepared by similar condensations using α-keto-acid derivs., di-Me acetylenedicarboxylate, and oxalate derivs. Two possible dual affinity inhibitors were also prepared The action of these compds. on yeast or Escherichia coli enzyme is discussed in relation to their bulk and electronic character.
ST riboflavin synthase inhibitor prepn
IT Molecular structure-biological activity relationship
(riboflavin synthase-inhibiting, of substrate and transition-state analogs)
IT 141-43-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with chloronitropyrimidinedione)
IT 100-34-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of diazotized, with ribitylaminopyrimidinedione)
IT 76641-69-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with diazotized benzenediazonium chloride)
IT 328-50-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with reduced dimethylmethylaminonitrosopyrimidinedione)
IT 762-42-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with hydroxyethylaminopyrimidinedione)
IT 34457-84-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitroribitylaminopyrimidinedione)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with reduced ethylaminonitropyrimidinedione)
IT 121-44-8, reactions 4755-77-5 6613-41-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with reduced hydroxyethylaminonitropyrimidinedione)
IT 52918-39-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloredn. of)
IT 4270-27-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitration of)
IT 5770-42-3 5770-44-5 6642-31-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitrosation of)
IT 6630-30-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with aminoethanol)
IT 61541-46-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with oxoglutaric acid)
IT 76641-72-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
IT 878-86-4P 1203-25-4P 76641-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with amines)
IT 76641-73-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with pyrimidines)
IT 620-79-1P 620-80-4P 5770-10-5P 52850-69-8P 76641-71-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 944-48-9P 4217-38-3P 6632-68-4P 7641-19-2P 18595-59-0P
33106-48-8P 66031-99-0P 66032-00-6P 76641-70-8P 76641-74-2P
76641-75-3P 76641-76-4P 76641-77-5P 76641-78-6P 76641-79-7P
76641-80-0P 76641-81-1P 76641-82-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 17801-83-1P 17879-89-9P 29161-67-9P 32507-81-6P 36075-32-8P
40773-79-3P 54367-34-9P 54367-35-0P 56677-30-6P 56677-31-7P
57821-16-6P 76641-32-2P 76641-33-3P 76641-34-4P 76641-35-5P
76641-36-6P 76641-37-7P 76641-38-8P 76641-39-9P 76641-40-2P

76641-41-3P 76641-42-4P 76641-43-5P 76641-44-6P **76641-45-7P**
76641-46-8P 76641-47-9P 76641-48-0P
76641-49-1P 76641-50-4P 76641-51-5P 76641-52-6P 76641-53-7P
76641-54-8P 76641-55-9P 76641-56-0P 76641-57-1P 76641-58-2P
76641-59-3P 76641-60-6P 76641-61-7P 76641-62-8P 76641-63-9P
76641-64-0P 76641-65-1P 76641-66-2P 76641-67-3P 76641-68-4P
76657-09-5P 76657-10-8P 76704-20-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and riboflavin synthase inhibition by, structure in relation to)

IT 100-52-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et acetoacetate)

IT 141-97-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzaldehyde)

IT 5770-52-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzylethylenedioxybutanal)

IT 527-47-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloropyrimidinedione)

IT 38087-02-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitropyrimidine; benzylmethylribitylpteridinedione by)

IT 134-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitropyrimidine, diphenylribitylpteridinedione by)

IT 122-51-0 34461-00-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ribitylaminopyrimidinedione)

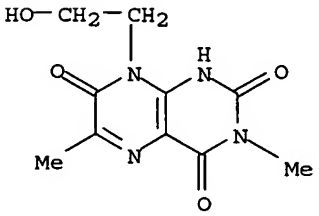
IT 26944-80-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

IT 36075-26-0 40773-76-0 50391-43-0 54367-37-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(riboflavin synthase inhibition by, structure in relation to)

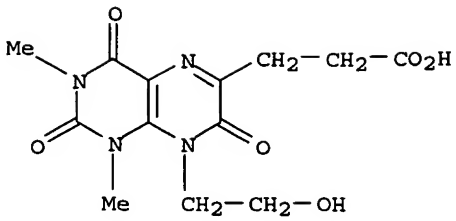
IT 9075-82-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(substrate and transition-state analogs inhibition of, structure in relation to)

IT **76641-45-7P 76641-46-8P 76641-47-9P**
76641-48-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and riboflavin synthase inhibition by, structure in relation to)

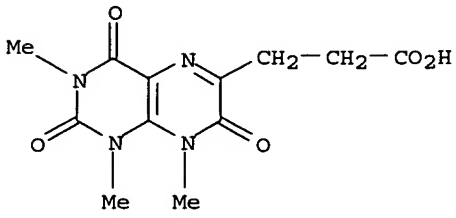
RN 76641-45-7 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 8-(2-hydroxyethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



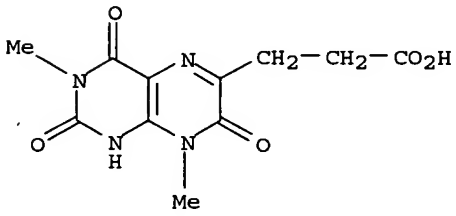
RN 76641-46-8 HCAPLUS
CN 6-Pteridinepropanoic acid, 1,2,3,4,7,8-hexahydro-8-(2-hydroxyethyl)-1,3-dimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)



RN 76641-47-9 HCAPLUS
CN 6-Pteridinepropanoic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)

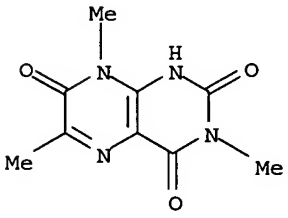


RN 76641-48-0 HCAPLUS
CN 6-Pteridinepropanoic acid, 1,2,3,4,7,8-hexahydro-3,8-dimethyl-2,4,7-trioxo- (9CI) (CA INDEX NAME)

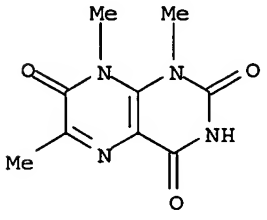


L59 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1979:456162 HCAPLUS
DN 91:56162
ED Entered STN: 12 May 1984
TI Interference between peri-substituents at positions 3 and 9 in purines and positions 1 and 8 in pteridines, shown by nuclear magnetic resonance spectroscopy. Proposal of a steric model
AU Bergmann, Felix; Tamir, Ilana; Frank, Arie; Pfleiderer, Wolfgang
CS Hahassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1979), (1), 35-9
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 22-9 (Physical Organic Chemistry)
AB NMR data are reported for 11 pteridine-2,4,7-triones and for 3 methoxypteridinediones. In 1,8-dimethylpteridine-2,4,7-triones, the chemical shifts of 1- and 8-Me substituents were shifted downfield by 0.12-0.18 ppm, due to steric interference. These downfield shifts are discussed in terms of spreading of the Me groups within the plane of the heterocyclic structure. The smaller change of δ values in pteridine-2,4,7-triones, as compared to reported values (B. et al., 1974) for purines, is explained in terms of partial lactimization of the 7,8- or 1,2-lactam

group in the 1- or 8-monomethyl derivs.
ST steric effect NMR pteridine
IT Nuclear magnetic resonance
(of pteridinetriones, steric effect on)
IT Steric effect
(on NMR of pteridinetriones)
IT 2577-38-0 2614-42-8 2614-43-9 2614-44-0 2622-65-3 2622-66-4
2625-21-0 **6743-26-6** 19845-00-2 70674-02-1 70916-39-1
70916-40-4
RL: PRP (Properties)
(NMR of)
IT **70916-41-5P** 70916-42-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
IT 70916-43-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of)
IT 7641-19-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction and condensation reactions of)
IT **6743-26-6**
RL: PRP (Properties)
(NMR of)
RN 6743-26-6 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)

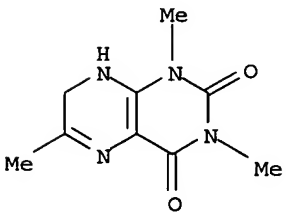


IT **70916-41-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 70916-41-5 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 1,6,8-trimethyl- (9CI) (CA INDEX NAME)

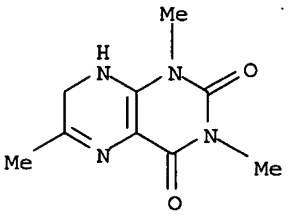


L59 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:115691 HCAPLUS
DN 66:115691
ED Entered STN: 12 May 1984
TI Synthesis of 6-hydroxymethyl-1,3-dimethyllumazine by rearrangement of the corresponding 6-methyllumazine 5-oxide
AU Zondler, Helmut; Forrest, Hugh S.; Lagowski, Jeanne M.
CS Univ. of Texas, Austin, TX, USA
SO Journal of Heterocyclic Chemistry (1967), 4(1), 124-6

CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 66:115691
GI For diagram(s), see printed CA Issue.
AB Starting with a chloronitrouracil, 1,3,6-trimethyllumazine (I) was prepared Oxidation to the 5-oxide and subsequent rearrangement gave 6-hydroxymethyl-1,3-dimethyllumazine. Because of the method of synthesis, the product is uncontaminated with the 7-isomer.
ST LUMAZINES; URACILS; PTERIDINES
IT Rearrangements
(of 1,3,6-trimethyllumazine 5-oxide to 6-(hydroxymethyl)-1,3-dimethyllumazine)
IT 14006-07-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)
IT 2625-21-0P 14005-09-5P 14005-10-8P 14006-04-3P **14006-05-4P** 14006-06-5P 14094-40-7P **14149-65-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **14006-05-4P 14149-65-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14006-05-4 HCAPLUS
CN Lumazine, 7,8-dihydro-1,3,6-trimethyl- (8CI) (CA INDEX NAME)



RN 14149-65-6 HCAPLUS
CN Lumazine, 7,8-dihydro-1,3,6-trimethyl-, monohydrochloride (8CI) (CA INDEX NAME)

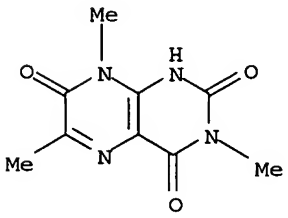


● HCl

L59 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1966:412315 HCAPLUS
DN 65:12315
OREF 65:**2260c-e**
ED Entered STN: 22 Apr 2001
TI Pteridine studies. XXXI. The covalent hydration and subsequent oxidation

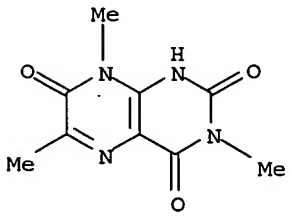
of 8-methyl derivatives of some amino- and hydroxypteridines
AU Jacobsen, N. W.
CS John Curtis School Med. Res., Australian Natl. Univ., Canberra
SO Journal of the Chemical Society [Section] C: Organic (1966), (12), 1065-72
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
AB cf. CA 64, 4891e. Pteridine derivs. with a C-Me substituent located at the site attacked by the hydroxyl group in the process of covalent hydration, are shown to undergo a facile demethylation when oxidized by KMnO4. Identification of the oxidation products (oxopteridines) by unambiguous syntheses served to establish the site of water addition in the original pteridines. Using this method, 2,8-dihydro-6,7,8-trimethyl-2-methyliminopteridine, 2,8-dihydro-6,7,8-tri-methyl-2-oxopteridine, and a series of related compds. were shown to undergo transmol. hydration at positions 1 and 7 (or 3 and 7) of the pteridine nucleus. The uv spectra of some unstable hydrated and anhydrous mols. are given, and these results are used to identify the stable hydrates of some heavily substituted pteridines which did not undergo oxidative dealkylation. The results of oxidation with other reagents, including xanthine oxidase, are reported.
IT Bases
IT Spectra, visible and ultraviolet
Spectra, visible and ultraviolet
(of pteridine derivs.)
IT Oxidation
(of pteridine derivs., hydration and)
IT Hydration (chemical)
(of pteridines, oxidation and)
IT 91-18-9, Pteridine
(derivs.)
IT 1603-79-8, Glyoxylic acid, phenyl-, ethyl ester 4388-87-8, 3,4-Hexanedione, 2,5-dimethyl- 6726-69-8, Pteridine, 2-amino-3,4-dihydro-4-methoxy-, hydrochloride 6726-70-1, Pteridine, 2-amino-3,4-dihydro-, compound with 2-amino-3,4-dihydro-4-pteridinol 6743-13-1, 7(8H)-Pteridinone, 2-methoxy-6,8-dimethyl- 6743-14-2, 7(8H)-Pteridinone, 2-hydroxy-6,8-dimethyl- 6743-15-3, 7(8H)-Pteridinone, 4-hydroxy-6,8-dimethyl- 6743-16-4, 4(8H)-Pteridinone, 8-methyl- 6743-17-5, 7(8H)-Pteridinone, 4-chloro-8-methyl- 6743-18-6, 7(8H)-Pteridinone, 4-hydroxy-8-methyl- 6743-19-7, 4(8H)-Pteridinone, 6-hydroxy-8-methyl- 6743-21-1, 2(8H)-Pteridinone, 6,7-diisopropyl-8-methyl- 6743-22-2, 2(8H)-Pteridinone, 8-methyl-6,7-diphenyl- 6743-24-4, 7(8H)-Pteridinone, 2-hydroxy-8-methyl-6-phenyl- 6743-25-5, 7(8H)-Pteridinone, 2,4-dihydroxy-6,8-dimethyl- 6743-26-6, 4,7(3H,8H)-Pteridinedione, 2-hydroxy-3,6,8-trimethyl- 6743-27-7, Pteridine, 2,8-dihydro-6,7,8-trimethyl-2-(methylimino)- 6743-28-8, 7(8H)-Pteridinone, 6,8-dimethyl-2-(methylamino)- 6743-29-9, Pteridine, 2,8-dihydro-6,7-diisopropyl-8-methyl-2-(methylimino)- 6743-30-2, 7(8H)-Pteridinone, 8-methyl-2-(methylamino)-6-phenyl- 6743-31-3, 7(8H)-Pteridinone, 6,8-dimethyl-4-(methylamino)- 6743-33-5, 2,7-Pteridinediol, 4-methyl- 6743-34-6, 2(8H)-Pteridinethione, 6,7,8-trimethyl- 6743-35-7, 7(8H)-Pteridinone, 2-mercapto-6,8-dimethyl- 6743-36-8, 2-Pyrimidinethiol, 5-amino-4-(methylamino)- 6743-38-0, Pteridine, 2-amino-3,4-dihydro-, p-toluenesulfonate 6743-39-1, Pteridine, 2-amino-3,4-dihydro- 6743-41-5, 1,3-Cyclohexanedione, 2-(2-amino-3,4-dihydro-4-pteridinyl)-5,5-dimethyl- 6743-42-6, 4,6-Pyrimidinediol, 5-(2-amino-3,4-dihydro-4-pteridinyl)- 6743-45-9, Pteridine, 2-amino-4-ethoxy-3,4-dihydro-, p-toluenesulfonate 6743-46-0, Pteridine, 2-amino-4-ethoxy-3,4-dihydro- 6743-47-1, Pteridine, 2-amino-4-ethoxy-3,4-dihydro-, hydrochloride 6758-42-5, Pteridine, 2-amino-3,4-dihydro-, picrate 6758-43-6, Pteridine, 2-amino-3,4-dihydro-4-(nitromethyl)- 6828-59-7, 7(8H)-Pteridinone, 4-chloro-6,8-dimethyl- 13530-12-6, 2(8H)-Pteridinone, 4-hydroxy-6,7-diisopropyl-8-methyl- 31937-02-7, 4-Pyrimidinol, 2-methyl-6-(methylamino)-5-nitro-
(preparation of)

IT 91-18-9, Pteridine
(spectrum of)
IT 6743-26-6, 4,7(3H,8H)-Pteridinedione, 2-hydroxy-3,6,8-trimethyl-
(preparation of)
RN 6743-26-6 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)



L59 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1966:412314 HCAPLUS
DN 65:12314
OREF 65:2260b-c
ED Entered STN: 22 Apr 2001
TI Structure of transient hydroperoxides in the autoxidation of reduced flavins
AU Mager, H. I. X.; Berends, W.
CS Inst. Technol., Delft, Neth.
SO Biochimica et Biophysica Acta (1966), 118(2), 440-1
CODEN: BBACAQ; ISSN: 0006-3002
DT Journal
LA English
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
AB cf. CA 64, 12676d. In studies on the spontaneous oxidation of tetrahydropteridines and reduced flavins leading to the formation of highly reactive hydroperoxides, the autoxidn. of 1,3,10-trimethyl-5,10-dihydroalloxazine was investigated. In the spontaneous oxidation of this compound in several anhydrous nonpolar solvents, 1 mole O was taken up per 2 moles reduced alloxazine. The product was identified as 3-oxo-1',3',4-tri-methyl - 1,2,3,4 - tetrahydroquinoxaline - 2 - spiro - 5' - hydantoin. This spirohydantoin was considered to be the ring opening-ring closure isomer of the corresponding hydroxyhydroalloxazine.
IT Oxidation
(aut-, of flavines, hydroperoxides and)
IT Hydroperoxides
(flavine autoxidn. in relation to)
IT Flavines (the isoalloxazine derivs.), adenine dinucleotide
(autoxidn. of, hydroperoxides and)
IT 1603-79-8, Glyoxylic acid, phenyl-, ethyl ester 4388-87-8, 3,4-Hexanedione, 2,5-dimethyl- 6743-13-1, 7(8H)-Pteridinone, 2-methoxy-6,8-dimethyl- 6743-14-2, 7(8H)-Pteridinone, 2-hydroxy-6,8-dimethyl- 6743-15-3, 7(8H)-Pteridinone, 4-hydroxy-6,8-dimethyl- 6743-16-4, 4(8H)-Pteridinone, 8-methyl- 6743-17-5, 7(8H)-Pteridinone, 4-chloro-8-methyl- 6743-18-6, 7(8H)-Pteridinone, 4-hydroxy-8-methyl- 6743-19-7, 4(8H)-Pteridinone, 6-hydroxy-8-methyl- 6743-21-1, 2(8H)-Pteridinone, 6,7-diisopropyl-8-methyl- 6743-22-2, 2(8H)-Pteridinone, 8-methyl-6,7-diphenyl- 6743-24-4, 7(8H)-Pteridinone, 2-hydroxy-8-methyl-6-phenyl- 6743-25-5, 7(8H)-Pteridinone, 2,4-dihydroxy-6,8-dimethyl- 6743-26-6, 4,7(3H,8H)-Pteridinedione, 2-hydroxy-3,6,8-trimethyl- 6743-28-8, 7(8H)-Pteridinone, 6,8-dimethyl-2-(methylamino)- 6743-30-2, 7(8H)-Pteridinone, 8-methyl-2-(methylamino)-6-phenyl- 6743-31-3, 7(8H)-Pteridinone, 6,8-dimethyl-4-(methylamino)- 6743-33-5, 2,7-Pteridinediol, 4-methyl- 6743-34-6, 2(8H)-Pteridinethione, 6,7,8-trimethyl- 6743-35-7, 7(8H)-Pteridinone, 2-mercapto-6,8-dimethyl-

6828-59-7, 7(8H)-Pteridinone, 4-chloro-6,8-dimethyl- 13530-12-6, 2(8H)-Pteridinone, 4-hydroxy-6,7-diisopropyl-8-methyl- 31937-02-7, 4-Pyrimidinol, 2-methyl-6-(methylamino)-5-nitro-
(preparation of)
IT 6743-26-6, 4,7(3H,8H)-Pteridinedione, 2-hydroxy-3,6,8-trimethyl-
(preparation of)
RN 6743-26-6 HCAPLUS
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)



L59 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1964:440465 HCAPLUS
DN 61:40465
OREF 61:7024h,7025a-b
ED Entered STN: 22 Apr 2001
TI Pyrido[2,3-d]pyrimidine-2,4,5,7-tetraones
IN Scarborough, Homer C.
PA Mead Johnson & Co.
SO 2 pp.
DT Patent
LA Unavailable
INCL 260256400
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI US 3139432		19640630	US	19630624	<--
GB 989048			GB		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 3139432	INCL	260256400	
US 3139432	NCL	544/279.000	<--

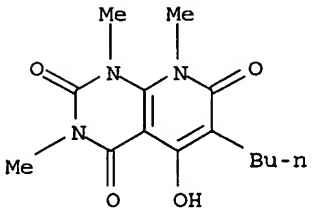
GI For diagram(s), see printed CA Issue.
AB Malonic acids are condensed with a 4-aminouracil in the presence of an acid anhydride to give compds. of the general formula I which can be used as bronchodilators. A mixture of 8.45 g. 1,3-dimethyl-4-(methylamino)uracil, 7.1 g. MeCH(CO2H)2, 11.3 ml. Ac2O, and 10 ml. HOAc is heated 2 hrs. on a steam bath, cooled, and filtered to give 48% 1,3,6,8-tetramethylpyrido[2,3-d]-pyrimidine-2,4,5,7-[1H,3H,6H,8H]-tetraone, m. 259.5-60.5° (MeCN). Similarly prepared are I(R = R1 = R2 = R3 = H),m. >360°; and the following I(R = R1 = Me)(R2,R3,and m.p. given): H, H, 280-2.5°; H, Me, 220.5-2.5°; Me, H, 287-9.5°; Bu, H, 195-6°; Bu, Me, 119-20°. Also prepared is the Na salt of I (R2 = H, R = R1 = R3 = Me).
IT Bronchi
(dilating substances for, pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrones as)
IT 271-80-7, 1H-Pyrazolo[3,4-d]pyrimidine 91996-75-7, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone
(derivs.)
IT 91996-75-7, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone 93117-35-2, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3-dimethyl- 93117-36-3, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3-dimethyl- 93738-66-0, Pyrido[2,3-d]pyrimidine-

2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,8-trimethyl- 93738-67-1, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6-trimethyl- 93738-68-2, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,8-trimethyl- 93738-69-3, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6-trimethyl- 95709-04-9, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 1,3,6,8-tetramethyl- 96732-25-1, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3-dimethyl- 96986-13-9, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3-dimethyl- **97360-49-1**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl- 97864-53-4, Pyrido[2,3-d]pyrimidine-2,4,5,7(1H,3H,6H,8H)-tetrone, 6-butyl-1,3,8-trimethyl-
(preparation of)

IT **97360-49-1**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl-
(preparation of)

RN 97360-49-1 HCAPLUS

CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl- (7CI) (CA INDEX NAME)



L59 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1964:440464 HCAPLUS

DN 61:40464

OREF 61:**7024f-h**

ED Entered STN: 22 Apr 2001

TI Tetrahydropyrimidinone

IN Boswell, George A.; Williams, Paul H.

PA Shell Oil Co.

SO 4 pp.

DT Patent

LA Unavailable

INCL 260251000

CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3137697		19640616	US	19620319 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3137697	INCL	260251000
US 3137697	NCL	544/315.000; 544/318.000; 564/048.000; 564/052.000; 564/057.000; 564/058.000; 564/059.000; 564/060.000 <--

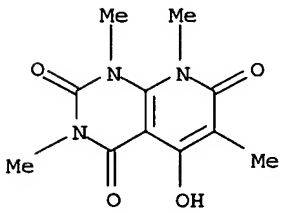
GI For diagram(s), see printed CA Issue.

AB Urea (120 g.) in iso-PrOH at 70° was treated dropwise with 147 cc. 93% acrolein, 90% of the acrolein was consumed in 30 hrs., and 1100 cc. of the reaction mixture was hydrogenated in the presence of 10-15 moles NH3 [to produce 1-(3-aminopropyl)urea] per mole of acrolein at 150° and 1500 lb./in.2 over 40 g. Raney Ni to yield 50 g. I, m. 250-5°. I and HCHO gave the 1,3-dimethylol derivative, m. 245-50°, which imparts crease-resistant properties to textiles.

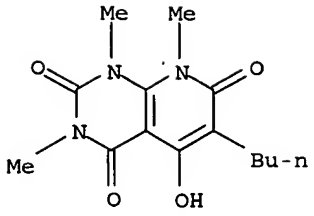
IT 1852-17-1, 2(1H)-Pyrimidinone, tetrahydro-
(manufacture of)

L59 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1964:45714 HCAPLUS
DN 60:45714
OREF 60:8027f-g
ED Entered STN: 22 Apr 2001
TI Pyrano[2,3-d]- and pyrido[2,3-d]pyrimidines
AU Scarborough, Homer C.
CS Mead Johnson Res. Center, Evansville, IN
SO Journal of Organic Chemistry (1964), 29(1), 219-21
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 60:45714
GI For diagram(s), see printed CA Issue.
AB The pyrano[2,3-d]pyrimidines (I) (R = H, Me) were prepared from 1,3-dimethylbarbituric acid and RCH(CO2H)2 in the presence of Ac2O and converted with EtOH, iso-PrOH, or aqueous NH4OH into II (R = EtO, iso-PrO, or NH2). Various III [R and R1 = H, Me, Me(CH2)2CH2] were prepared and shown by nuclear magnetic resonance spectroscopy to have the structure shown.
IT Nuclear magnetic resonance
(of pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)triones)
IT 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, δ-lactone
IT 254-61-5, Pyrido[2,3-d]pyrimidine 254-68-2, 2H-Pyrano[2,3-d]pyrimidine (derivs.)
IT 90559-74-3, 5-Pyrimidinepropionamide, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo- 92058-18-9, 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, ethyl ester 92848-56-1, 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, isopropyl ester 93117-36-3, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3-dimethyl- 93738-66-0, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,8-trimethyl- 93738-67-1, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6-trimethyl- **95709-05-0**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6,8-tetramethyl- 96986-13-9, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3-dimethyl- **97360-49-1**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl-
(preparation of)
IT **95709-05-0**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6,8-tetramethyl- **97360-49-1**, Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl-
(preparation of)
RN 95709-05-0 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6,8-tetramethyl- (7CI) (CA INDEX NAME)



RN 97360-49-1 HCAPLUS
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl- (7CI) (CA INDEX NAME)



L59 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1964:45713 HCAPLUS
DN 60:45713
OREF 60:8027c-f
ED Entered STN: 22 Apr 2001
TI O-Acylthiamine disulfides
AU Fujita, Tadashi; Mushika, Yoshitaka; Hagio, Katsuaki
CS Tanabe Seiyaku Co., Osaka, Japan
SO Yakugaku Zasshi (1963), 83, 1056-61
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
AB Thiamine disulfide (I)(4.2 g.) in 30 ml. H2O treated with 10% HCl with cooling, 10%NaOH added to pH 7, a solution of 6.7 g. NaS2O3Bz in 30 ml. CHCl3 added, the mixture kept alkaline by addition of 10% NaOH, the CHCl3 layer taken up in 20 ml. 5% HCl, the extract made alkaline with 10% NaOH and extracted with CHCl3, and 30 ml. C6H6 added to give 4.2 g. [RCH2N(CHO)CHMeC:C(CH2CH2OR')S]2 (II).C6H6.H2O (R = 2-methyl-4-amino-5-pyrimidyl throughout, R' = Bz) (III) (β-form), m. 148-9° (decomposition). III (3 g.) in CHCl3 passed through an Al2O3 column and concd, gave 1.8 g. III, m. 148-9° (decomposition); this in 13 vols. absolute EtOH concentrated gave II (R' = Bz) (α-form), m. 146-7°. I (11.2 g.) in 110 ml. C5H5N treated with 5.8 g. R'Cl (R' = 2-thenoyl) dropwise, the mixture stirred 2 hrs., kept overnight, and concentrated in vacuo, the residue in 100 ml. H2O made alkaline with 10% Na2CO3, the precipitate taken up in CHCl3, the CHCl3 layer concentrated, the residue treated with 100 ml. C6H6, and the product recrystd. (EtOH) gave 11.9 g. II (R' = 2-thenoyl) (IV) (α-form), m. 144-5°. A mixture of 5 g. Na2S2O3.5H2O, 2.9 g. 2-thenoyl chloride, 6 ml. H2O, and 6 ml. EtOH kept 20 min. at 12°, treated with 6 g. I and the product worked up as above gave 3.3 g. II.C6H6.H2O (R' = 2-thenoyl) (V) (β-form), m. 145-7° (decomposition). Recrystn. of V from 10 vols. absolute EtOH gave II (R' = 2-thenoyl) (α-form), m. 144-5°. Similarly, 11.2 g. I and 5.2 g. 2-furoyl chloride was treated as for III to give 12.1 g. II.H2O (R' = 2-furoyl) (VI) (α-form), m. 119-20° (EtOH). Alternatively, reaction of 5 g. Na2S2O3.5H2O, 2.6 g. 2-furoyl chloride, 6 ml. H2O, and 6 ml. EtOH and the product treated with 6 g. I gave 3.2 g. VI.C6H6.H2O (β-form), m. 128-9° (decomposition). VI.-2HCl.2H2O m. 182-3° (decomposition); picrate m. 148-50° (de-composition).
IT 2-Thiophenecarboxylic acid, diester with N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide], dihydrochloride
2-Thiophenecarboxylic acid, diester with N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide], isomers
5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, δ-lactone
IT 67-16-3, Formamide, N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-(esters)
IT 2667-89-2, Formamide, N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-, dibenzoate 2667-89-2, Formamide, N,N'-[dithiobis[2-(2-hydroxyethyl)-1-

methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-, dibenzoate 5008-09-3, 2-Furoic acid, diester with N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide]
(isomers)

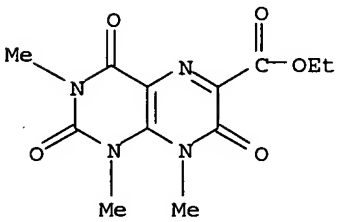
IT 89418-39-3, Thiocyanic acid, 2-amino-6-methyl-4-pyrimidinyl ester 89580-22-3, Thiocyanic acid, 4-amino-6-methyl-2-pyrimidinyl ester 89937-98-4, Thiocyanic acid, 6-methyl-2-(methylthio)-4-pyrimidinyl ester 90916-08-8, 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-α,1,3-trimethyl-β,2,4-trioxo-, δ-lactone 90993-13-8, Thiocyanic acid, chloromethylpyrimidinyl ester 91347-74-9, Thiocyanic acid, 2-(3,5-dimethylpyrazol-1-yl)-6-methyl-4-pyrimidinyl ester 92058-18-9, 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, ethyl ester 92295-53-9, Thiocyanic acid, 2-(3,5-dimethylpyrazol-1-yl)-5,6,7,8-tetrahydro-4-quinazolinyl ester 92848-56-1, 5-Pyrimidinepropionic acid, 1,2,3,4-tetrahydro-6-hydroxy-1,3-dimethyl-β,2,4-trioxo-, isopropyl ester 96620-52-9, Thiocyanic acid, 2-(3,5-dimethylpyrazol-1-yl)-6,7-dihydro-5H-cyclopentapyrimidin-4-yl ester 106194-16-5, 2-Furoic acid, diester with N,N'-[dithiobis[2-(2-hydroxy-ethyl)-1-methylvinylene]]bis[N-(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide], dihydrochloride 106784-85-4, 2-Thiophenecarboxylic acid, diester with N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide], dipicrate 106784-86-5, 2-Furoic acid, diester with N,N'-[dithiobis[2-(2-hydroxyethyl)-1-methylvinylene]]bis[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamide], dipicrate
(preparation of)

L59 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1962:442844 HCAPLUS
DN 57:42844
OREF 57:8569f-i,8570a-i
ED Entered STN: 22 Apr 2001
TI Pteridines. XXI. The synthesis and structure of 8-substituted 2,4,7-trioxohexahydropteridine-6-carboxylic acids
AU Nuebel, Gotthard; Pfleiderer, Wolfgang
CS Tech. Hochschule, Stuttgart, Germany
SO Ber. (1962), 95, 1605-14
DT Journal
LA Unavailable
CC 32 (Heterocyclic Compounds-More than One Hetero Atom)
AB Various 8-alkyl derivs. (I) of 2,4,7-trioxohexahydropteridine-6-caboxylic acid (II) and of the Et ester (III) of II were synthesized. The comparison of their spectra indicates that the N-1-atom, not the CO2H, carries the most acidic H. The dissociation sequence of the acidic H atoms in the I is N-1 > CO2H > N-3. 5-Amino-4-ethylaminouracilHCl (IV) (2 g.) in 30 cc. H2O adjusted with alkali to pH 6, refluxed 0.5 hr. with 3 g. CO(CO2Et)2.H2O (V.H2O), cooled, and filtered yielded 1 g. Et ester (VI) of the 8-Et derivative (VII) of II, needles, m. 275° (H2O). VI (1.7 g.) in 20 cc. N NaOH refluxed 0.5 hr., treated with C, acidified hot with 5N HCl, and filtered after several hrs. gave 1.1 g. VII, m. above 330°. 4-(2-HOCH2CH2) analog (VIII) (1 g.) of IV in 20 cc. H2O and 2 g. V.H2O refluxed 0.5 hr., cooled, and filtered, and the residue refluxed with 15 cc. N NaOH and acidified with 5N HCl gave 0.6 g. yellowish 8-(2-HOCH2CH2) derivative (IX) of II, m. 222° with foaming. IX (0.5 g.) in 30 cc. MeOH refluxed to solution with 0.5 cc. concentrated H2SO4, and then 1 addnl. hr., treated with C, and diluted with H2O yielded 0.3 g. yellowish Me ester (X) of IX, m. 287° (MeOHHCONMe2). 5-Amino-4-benzylaminouracil-HCl (XI) (1.5 g.) in 30 cc. H2O refluxed 0.5 hr. with 3 g. V.H2O, cooled, and filtered, and the residue boiled with 20 cc. N NaOH and acidified with 5N HCl gave 1 g. yellowish 8-PhCH2 derivative (XII) of II, m. 268°. XII(1 g.), 70 cc. MeOH, and 3 cc. concentrated H2SO4 gave in the usual manner 0.7 g. yellowish Me ester (XIII) dihydrate of XII, m. 261-2°, which dried in vacuo at 110° over P2O5 gave XIII. 3-Methyl-5-nitroso-4-methylaminouracil (1.8 g.) in 50 cc. H2O hydrogenated over Raney Ni, boiled briefly, filtered hot, refluxed 15 min.

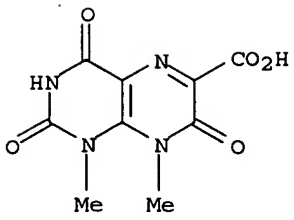
with 2 g. V, refrigerated overnight, and filtered gave 1.2 g. Et ester (XIV) of the 1,8-di-Me derivative (XV) of II, m. 275-7° (H2O). XIV (0.6 g.) and 10 cc. 0.5N NaOH refluxed 10 min., acidified with 5N HCl to pH 0, cooled, kept overnight, and filtered yielded 0.4 g. XV, m. 220° with foaming. N-Methylbarbituric acid (12 g.), 4 cc. H2O, and 96 cc. POCl3 refluxed 0.5 hr. and evaporated, and the sirupy residue poured onto ice and filtered gave 8 g. 1-methyl-4-chlorouracil (XVI), m. 276-7° (H2O). XVI (1 g.) and 5 g. PhCH2NH2 refluxed 1 hr., cooled, diluted with H2O, and filtered, and the dried residue (1.13 g.) recrystd. from 170 cc. EtOH gave 0.85 g. 4-PhCH2NH analog (XVII) of XVI, m. 282° with sintering from 260°. XVII (0.5 g.) in 100 cc. EtOH hydrogenated 17 hrs. at 38° over 1 g. Pd-C, filtered, and evaporated gave 0.24 g. 4-NH2 analog of XVI, m. 330° (H2O). XVI (5 g.) and 10 cc. liquid MeNH2 heated 1 hr. at 120° in a sealed tube and evaporated, and the residue dissolved in H2O, acidified with AcOH, and refrigerated overnight gave 3.2 g. 4-MeNH analog (XVIII) of XVI, m. 290° (H2O). XVIII (1 g.) in 20 cc. H2O treated at 90° with 0.5 g. NANO2, acidified with AcOH, and cooled gave 0.8 g. red 5-NO derivative of XVIII, m. 267° (decomposition). XVII (2 g.) in 200 cc. H2O treated with 1 g. NANO2 and acidified with AcOH gave 2 g. orange-red 5-NO derivative (XIX) of XVII, decomposed at 188°. XVII (2.4 g.) in 60 cc. boiling H2O treated with 1 g. NaNO2, acidified, cooled, and filtered, the residual XIX dissolved in 60 cc. HCO2H, treated with 4 g. Zn dust in portions, refluxed 0.5 hr., cooled, and filtered, the filtrate evaporated, and the residue treated with hot H2O gave 2 g. 5-OHCNH derivative (XX) of XVII, m. 238° (aqueous HCO2H). XX (2 g.) in 50 cc. HCl-MeOH refluxed 1 hr. gave 1.4 g. 1-methyl-5-amino-4-benzylaminouracil-HCl (XXI), m. above 330°. XXI (2 g.) and 1.6 g. V in 20 cc. H2O heated 15 min. on the water bath and filtered yielded 1.4 g. Et ester (XXII) of the 3-methyl-8-benzyl derivative (XXIII) of II, m. 177° (aqueous EtOH). XXII (1 g.) and 15 cc. N Na2CO3 refluxed 0.5 hr., treated with C, acidified hot with 5N HCl, cooled, and filtered gave 0.5 g. yellowish XXIII, m. 188-90° with foaming (EtOH containing a few drops 5N HCl). IV (1.5 g.) in 40 cc. H2O adjusted to pH 6, treated with 3 cc. EtO2CCH(OH)OEt (XXIV), and filtered, and the residue refluxed 0.5 hr. with 50 cc. N NaHCO3, acidified with 5N HCl, and cooled gave 0.9 g. yellowish 8-ethyl-2,4,7-trioxohexahydropteridine (XXV), m. above 340° (H2O). VIII and 4 cc. XXIV gave similarly 1.5 g. yellowish 8-(2HOCH2CH2) analog (XXVI) of XXV, m. 326° (H2O). XXVI (0.5 g.) in 30 cc. AC2O refluxed 6 hrs. and cooled gave 0.3 g. acetate (XXVII) of XXVI, m. 273° with subsequent resolidification (H2O). XI (2 g.) and 4 cc. XXIV gave in the usual manner 1.6 g. 8-PhCH2 analog (XXVIII) of XXV, m. 288° (decomposition) (H2O). The Rf values were determined with 2:1 BuOH-5N AcOH, 2:1 PrOH-1% NH3, 4% aqueous Na citrate, and 3% aqueous NH4Cl (given in this order for the following compds.: VI, 0.30, 0.58, 0.52, 0.61; II, 0.11, 0.11, 0.62, 0.58; IX, 0.06, 0.07, 0.64, 0.65; X, 0.12, 0.35, 0.48, 0.57; XII, 0.23, 0.27, 0.61, 0.63; XIII, 0.39, 0.63, 0.48, 0.57; XIV, 0.38, 0.34, 0.57, 0.61; XV, 0.23, 0.19, 0.70, 0.66; XXII, 0.68, 0.70, 0.78, 0.78; XXIII, 0.50, 0.41, 0.54, 0.58; XXV, 0.26, 0.44, 0.47, 0.60; XXVI, 0.13, 0.28, 0.50, 0.61; XXVII, 0.27, 0.48, 0.56, 0.68; XXVII, 0.42, 0.63, 0.50, 0.59; 1,3,6-trimethyl-7-hydroxy-2,4-dioxotetrahydropteridine, 0.70, 0.50, 0.50, 0.60. The pK values in H2O at 20° were determined for the following compds.: 8-Me derivative of II, 2.15 ± 0.1, 4.72 ± 0.02, 13.06 ± 0.1; VI, 2.93 ± 0.1; II, 2.28 ± 0.1, 4.85 ± 0.03, 13.1 ± 0.1; IX, 1.94 ± 0.1, 4.78 ± 0.02, 12.6 ± 0.1; X, 2.65 ± 0.1; XII, 1.69 ± 0.1, 4.77 ± 0.03, 12.9 ± 0.1; XIII, 2.06 ± 0.05; XIV, 7.74 ± 0.04; XV, 2.22 ± 0.1, 8.54 ± 0.1; Et 1,3,8-trimethyl2,4,7-trioxohexahydropteridine-6-carboxylate, 2.82 ± 0.03; XXII, 2.16 ± 0.06; XXIII, 1.65 ± 0.1, 4.58 ± 0.1; 8methyl-2,4,7-trioxohexahydropteridine, 3.80 ± 0.01, 12.85 ± 0.1; XXV, 3.87 ± 0.01, 13.02 ± 0.1; XXVI, 3.51 ± 0.03, 12.79 ± 0.1; XXVII, 3.20 ± 0.03; XXVIII, 3.05 ± 0.06, 12.98 ± 0.1. The ultraviolet absorption maximum of the various 8-alkyl derivs. of I and II are tabulated.

IT Spectra, visible and ultraviolet
(of 1,2,3,4,7,8-hexahydro-6-pteridinecarboxylic acid derivs.)

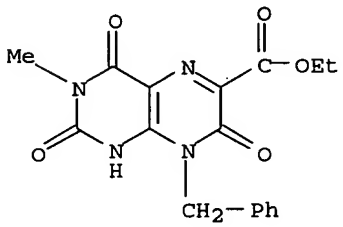
IT Spectra, visible and ultraviolet
(of pteridine derivs.)
IT 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-3-methyl-2,4,7-trioxo-
IT 19845-00-2, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-methyl- 90321-74-7, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-8-methyl-2,4,7-trioxo- **91769-67-4**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester
(acidity of)
IT 33744-31-9, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-2,4,7-trioxo-
(derivs.)
IT 4318-56-3, Uracil, 6-chloro-3-methyl- 5759-63-7, Uracil, 3-methyl-6-(methylamino)- 5759-79-5, Uracil, 6-(benzylamino)-3-methyl- 5770-19-4, Uracil, 3-methyl-6-(methylamino)-5-nitroso- 5770-20-7, Uracil, 6-(benzylamino)-3-methyl-5-nitroso- 17801-82-0, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-(2-hydroxyethyl)- 21236-97-5, Uracil, 6-amino-3-methyl- 70404-26-1, Formamide, N-[4-(benzylamino)-1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-5-pyrimidinyl]- 89977-69-5, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-ethyl- 90324-11-1, 6-Pteridinecarboxylic acid, 8-ethyl-1,2,3,4,7,8-hexahydro-2,4,7-trioxo- **90324-12-2**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo- 90324-20-2, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-8-(2-hydroxyethyl)-2,4,7-trioxo- 90917-19-4, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-(2-hydroxyethyl)-, acetate 91141-83-2, 6-Pteridinecarboxylic acid, 8-ethyl-1,2,3,4,7,8-hexahydro-2,4,7-trioxo-, ethyl ester 91687-86-4, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-8-(2-hydroxyethyl)-2,4,7-trioxo-, methyl ester 91823-54-0, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-benzyl- 92061-33-1, 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-2,4,7-trioxo- **93318-04-8**, 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-3-methyl-2,4,7-trioxo-, ethyl ester **95296-09-6**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo-, ethyl ester 95766-75-9, Uracil, 5-amino-6-(benzylamino)-3-methyl-, hydrochloride 820996-74-5, 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-2,4,7-trioxo-, methyl ester
(preparation of)
IT **91769-67-4**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester
(acidity of)
RN 91769-67-4 HCAPLUS
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester (6CI, 7CI) (CA INDEX NAME)



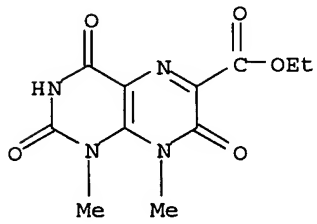
IT **90324-12-2**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo- **93318-04-8**, 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-3-methyl-2,4,7-trioxo-, ethyl ester **95296-09-6**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo-, ethyl ester
(preparation of)
RN 90324-12-2 HCAPLUS
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo- (7CI) (CA INDEX NAME)



RN 93318-04-8 HCAPLUS
CN 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-3-methyl-2,4,7-trioxo-, ethyl ester (7CI) (CA INDEX NAME)



RN 95296-09-6 HCAPLUS
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo-, ethyl ester (7CI) (CA INDEX NAME)



L59 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1959:7096 HCAPLUS
DN 53:7096
OREF 53:**1364f-i,1365a-i,1366a**
ED Entered STN: 22 Apr 2001
TI Pteridines. VII. Methylations of hydroxypteridines
AU Pfleiderer, Wolfgang
CS Tech. Hochschule, Stuttgart, Germany
SO Chemische Berichte (1958), 91, 1671-80
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
AB cf. C.A. 52, 18457h. The stepwise methylation of 7-hydroxy-2,4-dioxotetrahydropteridine (I) and its 6-Me derivative (II) shows differences in the sequence of the substitutions and of the dissociation of the acidic H (determined spectrophotometrically). Steric factors seem to be responsible for this different behavior. II (1.8 g.) in 40 cc. 0.5N KOH treated dropwise at 40° with stirring with 2 cc. Me2SO4 while maintaining a pH of 9 by the dropwise addition of N KOH, the mixture acidified strongly with HCl, refrigerated overnight, and filtered by suction, and the residue recrystd. from H2O with C yielded 1 g. 8-methyl-2,4,7-trioxohexahydropteridine (III), m. above 350°; the filtrate extracted 16 hrs. with CHCl3 yielded

0.3 g. 1,3-di-Me derivative (IIIa) of I. III (1 g.) in 20 cc. N NaOH treated at 60° with stirring dropwise with 2 cc. Me2SO4 in 2 cc. MeOH, cooled slowly to 40°, kept at pH 9 by the addition of 5N NaOH, acidified with 5N HCl to pH 1, refrigerated overnight, and filtered yielded 0.4 g. 3-Me derivative (IV) of III, pale yellow crystals, m. above 350° with browning from 300°. 3-Me derivative (2.2 g.) (V) of I in 25 cc. 0.5N KOH treated at 40° with stirring dropwise with 4 cc. Me2SO4, the mixture kept at pH 9 with 2N KOH, and the product isolated in the usual manner yielded 0.5 g. IV; the filtrate evaporated and recrystd. from H2O yielded 0.2 g. IIIa; the reaction filtrate extracted 24 hrs. with CHCl3 gave 0.4 g. IIIa, m. 264°; the CHCl3 extract evaporated and the residue recrystd. from a little H2O with C yielded 0.2 g. 7-MeO analog of IIIa, m. 195°. 3,8-Dimethyl-2-methylthio-4,7-dioxotetrahydropteridine (VI) (0.6 g.) refluxed 5 hrs. with 12 cc. 5N H2SO4, diluted with 12 cc. H2O, treated with C, and refrigerated 3 days gave 0.3 g. mixture of IV and VI; a 0.3-g. portion treated with 10 cc. cold 0.1H NH4OH, filtered with suction, acidified with N HCl, refrigerated, and filtered, and the residue boiled with a little EtOH, filtered hot, and recrystd. from H2O yielded 0.06 g. IV. 1-Methyl-2-methylthio-4,5-diamino-6-oxodihydropyrimidine (6 g.) in 200 cc. H2O, cooled to room temperature, treated with 6 g. EtO2CCH(OH)OEt (VII), and filtered after 1 hr. gave 8 g. 1-methyl-2-methylthio-4-amino-6-oxodihydropyrimidine-5-azomethinecarboxylic acid Et ester (VIII), pale yellow crystals, m. 178° resolidified at 180° (EtOH). VIII (8 g.) refluxed with 200 cc. 0.5N NaHCO3 0.5 hr., treated with C, acidified in the heat to pH 1, cooled, and filtered gave 4.5 g. 3-methyl-2-methylthio-4,7-dioxotetrahydropteridine (IX), m. 292-4° (decomposition) (H2O). IX (4.5 g.) in 40 cc. N KOH treated at 40° with stirring dropwise with 4 cc. Me2SO4 and 5N KOH at pH 9, acidified with AcOH, refrigerated several hrs., and filtered, and the residue recrystd. from H2O yielded 3.2 g. VI, m. 239°. IX (0.2 g.) refluxed 2 hrs. with 10 cc. N H2SO4, kept several hrs., and filtered gave 0.08 g. V. 1-Me derivative (X) (2.1 g.) of III in 25 cc. H2O adjusted with N KOH to pH 9, treated dropwise at 40° with 1.5 cc. Me2SO4 and N KOH with stirring, and filtered, the residue dissolved in H2O, and the solution acidified gave 0.9 g. unchanged X; the filtrate adjusted with 5N HCl to pH 0 and refrigerated several hrs. gave 0.8 g. IIIa, m. 264° (H2O). 3-Phenyl-4,5-diaminouracil (XI) (8.8 g.) in 200 cc. H2O treated with stirring with 8 g. VII, filtered after 2 hrs., treated with 120 cc. N NaHCO3, refluxed 0.5 hr., treated with C, and acidified with 5N HCl yielded 4.5 g. 1-Ph derivative (XII) of III, m. above 360° (H2O). 1-Me derivative (4.6 g.) of XI in 200 cc. H2O treated with 6 g. VII and filtered after 2 hrs. gave 5.2 g. 1-methyl-3-phenyl-4-aminouracil-5-azomethinecarboxylic acid Et ester (XIII), pale yellow crystals, m. 206-7°. XIII (5 g.) refluxed 0.5 hr. with 100 cc. NaHCO3, acidified with 5N HCl, cooled, and filtered, and the residue repptd. from base with acid gave 3.1 g. 3-Me derivative (XIV) of XII, m. 362° (glacial AcOH). XII (2.5 g.) in 15 cc. 2N NaOH treated with stirring at 40° dropwise with 5 cc. Me2SO4 and 5N NaOH at pH 9, cooled, and filtered, the filtrate acidified, the precipitate filtered off and repptd. from hot base with acid gave XIV; the 1st filter residue treated with dilute NH4OH and filtered, and the filtrate acidified at reflux temperature gave addnl. XIV (total 1.2 g.); the NH4OH-insol. filter residue recrystd. from EtOH with C gave 0.5 g. 7-MeO analog (XV) of XIV, m. 254°. XII (1 g.) in 75 cc. absolute MeOH treated with CH2N2 [from 10 g. H2NCON(NO)Me] in Et2O, allowed to stand 1 hr., and filtered, the filtrate evaporated, and the residue recrystd. from aqueous EtOH yielded 0.6 g. XV, m. 254°. II (1 g.) in 35 cc. H2O dissolved with warming with the addition of 6 cc. N KOH, cooled to 40°, treated dropwise with stirring with 1 cc. Me2SO4 in 2 cc. MeOH, maintained with 2N KOH at about pH 9, acidified to pH 1, and filtered from 0.25 g. solid, the filtrate concentrated to half-volume, refrigerated 1 day, and filtered, and the residue recrystd. from H2O gave 0.45 g. 6-Me derivative (XVI) of III, m. above 350°. XVI (1.5 g.) in 40 cc. N NaOH treated at 75° dropwise with stirring with 5 cc. Me2SO4 while being kept at pH 10-12 with 5N NaOH, acidified with N HCl to pH 1, cooled, and filtered gave 1.1 g. 3-Me derivative (XVII) of XVI, m. 331-4° (EtOH). XVII (0.5 g.) in 10 cc. absolute MeOH treated with

CH2N2 in Et2O, filtered after 3 hrs., and recrystd. from MeOH yielded 0.35 g. 3,6,8-trimethyl-2-methoxy-4,7-dioxotetrahydropteridine (XVIII), m. 243° (MeOH). 1,6-Di-Me derivative (XIX) (1.2 g.) of I in 20 cc. H2O treated with 6 cc. N KOH and then with stirring at 40° with 1 cc. Me2SO4 in 3 cc. MeOH, adjusted with N KOH to pH 9, acidified with 5N HCl, allowed to stand several hrs., and filtered gave 0.8 g. 3-Me derivative (XX) of XIX, m. 308°. The Rf values in 2:1 BuOH-5N AcOH, 2:1 PrOH-1% NH3, 4% aqueous Na citrate, and 3% aqueous NH4Cl, the pK values at 20° in H2O, and the pH values of the neutral mol. and the monoanion were determined for the following compds.: IV, 0.29, 0.48, 0.45, 0.58, 3.83 ± 0.03, 1.5, 6.0; XVII, 0.42, 0.50, 0.47, 0.56, 4.22 ± 0.03, 2.0, 6.5; XVIII, 0.73, 0.65, 0.74, 0.75, -, 6.0, -; XII, 0.55, 0.43, 0.50, 0.63, 2.95 ± 0.05 (9.46 ± 0.04), 0.7, 6.2 (12.0 dianion); XIV, 0.73, 0.57, 0.62, 0.75, 3.49 ± 0.05, 1.2, 5.8; XV, 0.86, 0.72, 0.71, 0.75, -, 6.0, -; IX, 0.50, 0.46, 0.37, 0.51, 6.47 ± 0.04, 4.2, 8.7; VI, 0.56, 0.52, 0.57, 0.58, -, 6.0, -; XX, 0.70, 0.50, 0.50, 0.60, -, -, -. The fluorescence colors of the various pteridine derivs. are tabulated. The ultraviolet absorption spectra of the neutral mols. of IV, XVII, and XVIII and of the monoions of III, IV, XVII, and XVIII are recorded.

IT Steric effects or Steric factors
(in methylation of hydroxypteridines)

IT Methylation
(of 7-pteridinols)

IT Fluorescence
Ultraviolet and visible, spectra
(of pteridine derivs.)

IT 91-18-9, Pteridine
(derivs.)

IT 2432-27-1, 7-Pteridinol
(derivs., methylation of)

IT 31053-46-0, Lumazine, 7-hydroxy-6-methyl-
(methylation of)

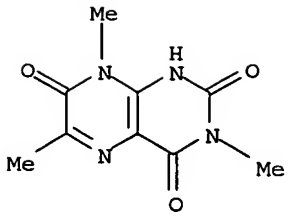
IT 2577-38-0, Lumazine, 7-hydroxy-
(of methylation)

IT 2614-42-8, Lumazine, 7-methoxy-1,3-dimethyl- 2614-43-9, Lumazine, 7-hydroxy-1,3-dimethyl- 2622-65-3, Lumazine, 7-hydroxy-3-methyl- 2625-21-0, Lumazine, 7-hydroxy-1,3,6-trimethyl- 6743-25-5, 2,4,7(1H,3H,8H)-Pteridinetrione, 6,8-dimethyl- 6743-26-6, 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- 19845-00-2, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-methyl- 70916-39-1, 2,4,7(1H,3H,8H)-Pteridinetrione, 3,8-dimethyl- 70916-40-4, 4,7(3H,8H)-Pteridinedione, 2-methoxy-3,6,8-trimethyl- 99587-06-1, Formic acid, {N-[4-amino-1,6-dihydro-1-methyl-2-(methylthio)-6-oxo-5-pyrimidinyl]formimidoyl}-, ethyl ester 100974-92-3, Formic acid, [N-(6-amino-1,2,3,4-tetrahydro-3-methyl-2,4-dioxo-1-phenyl-5-pyrimidinyl)formimidoyl]-, ethyl ester 102589-22-0, 4,7(3H,8H)-Pteridinedione, 3,8-dimethyl-2-(methylthio)- 108128-89-8, 4,7(3H,8H)-Pteridinedione, 3-methyl-2-(methylthio)- 108989-62-4, Lumazine, 7-hydroxy-3-methyl-1-phenyl- 109187-19-1, Lumazine, 7-methoxy-3-methyl-1-phenyl- 110251-58-6, Lumazine, 7-hydroxy-1-phenyl-
(preparation of)

IT 6743-26-6, 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl-
(preparation of)

RN 6743-26-6 HCAPLUS

CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)



L59 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1959:7095 HCAPLUS
DN 53:7095
OREF 53:1364b-f
ED Entered STN: 22 Apr 2001
TI SN-Reactions on the sulfonyl group of arylsulfonic acid derivatives. III. A method for the separation of secondary amines by alcoholate cleavage of sulfonamides
AU Klamann, Dieter; Bertsch, Helmuth
CS Tech. Univ., Berlin, Germany
SO Chemische Berichte (1958), 91, 1688-90
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
AB Mixts. of N,N-dialkyl, N-alkyl-N-aryl, and N,N-diarylamines can be separated by treatment of their sulfonic acid derivs. with alcoholates because only aromatically substituted compds. are cleaved to the free amine. The unreactivity of the sulfonamides of primary amines towards alcoholates allows a modification of the Hinsberg method for the separation of primary and secondary amines in cases where the alkali salt of the primary sulfonamide is difficultly soluble p-MeC6H4SO2N(C12H25)2 (I) (5.08 g.) and 6.47 g. p-MeC6H4SO2NPh2 refluxed 3 hrs. with 150 cc. 42% iso-AmONa, the mixture decomposed in the usual manner, the alc. phase treated with HCl and steam distilled, the distillation residue basified and again steam distilled, and the distillate filtered after 12 hrs. yielded 3.12 g. Ph2NH, m. 53°; the distillation residue acidified and extracted with petr. ether gave 5.08 g. unchanged I. p-MeC6H4SO2NEtC8H17 (II) (6.23 g.) and 5.51 g. p-MeC6H4SO2NHEt stirred 6 hrs. with 150 cc. 51% iso-AmONa, acidified, steam distilled, basified, steam distilled, the distillate treated with alkali and extracted with petr. ether, and the extract treated with HCl and evaporated gave 2.66 g. PhNHEt.HCl; the steam distillation residue. extracted with petr. ether, the extract dried, chromatographed on Al2O3, and eluted with EtOH yielded 5.06 g. unchanged II, n20D 1.5045. N,N-Dicyclohexyl-p-toluenesulfonamide (III) (3.35 g.) and 6.47 g. p-MeC6H4SO2NPh2 treated 2 hrs. with 150 cc. 42% iso-AmONa and worked up in the usual manner gave 2.85 g. Ph2NH; the steam distillation residue filtered gave 3.32 g. unchanged III, m. 118°. N-(2-Naphthyl)-p-toluenesulfonamide (IV) (5.95 g.) and 6.51 g. N-Et derivative of IV refluxed 6 hrs. with stirring with 150 cc. 51% iso-AmONa and the mixture worked up in the usual manner gave 4.05 g. 2-C10H7NHEt.HCl, m. 236°; the steam distillation residue heated some time with HCl and filtered gave 5.95 g. IV, m. 132-2.5° (EtOH).
IT Alcoholates
(of sulfonamides, in separation of secondary amines)
IT Amines
(separation of secondary)
IT Sulfonamides
(separation of secondary amines as)
IT p-Toluenesulfonamide, N-ethyl-N-octyl-
(alcoholysis of)
IT 80-39-7, p-Toluenesulfonamide, N-ethyl- 18271-18-6, p-Toluenesulfonamide, N-2-naphthyl- 39830-56-3, p-Toluenesulfonamide, N,N-dicyclohexyl- 79130-50-0, p-Toluenesulfonamide, N,N-didodecyl- 86488-48-4, p-Toluenesulfonamide, N-ethyl-N-2-naphthyl-

(alcoholysis of)
IT 63019-15-8, 2-Naphthylamine, N-ethyl-, hydrochloride
(formation by cleavage of p-toluenesulfonamides)
IT 4348-19-0, Aniline, N-ethyl-, hydrochloride
(formation from cleavage of p-toluenesulfonamides)
IT 3007-31-6, Didodecylamine 4088-36-2, Octylamine, N-ethyl-
(formation from cleavage of p-tolylsulfonyl derivs.)
IT 122-39-4, Diphenylamine
(formation of, from cleavage of N-p-tolylsulfonyl derivs.)
IT 101-83-7, Dicyclohexylamine
(formation of, from cleavage of p-tolylsulfonyl derivs.)

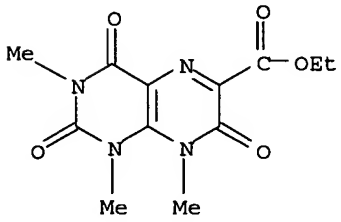
L59 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1958:104360 HCAPLUS
DN 52:104360
OREF 52:18459f-i,18460a
ED Entered STN: 22 Apr 2001
TI Pteridines. IV. 7-Hydroxy-2,4-dioxotetrahydropteridine-6-carboxylic acids
AU Pfleiderer, Wolfgang
CS Tech. Hochschule, Stuttgart, Germany
SO Chemische Berichte (1957), 90, 2617-23
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
OS CASREACT 52:104360
AB Spectra show H-bonding between CO2H and 7-OH in the acids and monoanions, the order of ionization is CO2H, 7-OH, N1-H, N3-H. 4,5-Diaminouracil (1.8 g.) refluxed 20 min. with 4 g. (HO)2C(CO2Et)2.H2O (I) in 150 cc. H2O, aged, and filtered, then refluxed 15 min. with 50 cc. N NaOH, diluted with H2O to clear solution at b.p., then added to 150 cc. boiling 0.5N HCl, gives 1.8 g. 7-hydroxy-2,4-dioxotetrahydropteridine-6-carboxylic acid. Similarly the 1-Me and 3-Me derivs. are prepared 5-Nitroso-4 -methylaminouracil (1.2 g.) reduced by alkaline Na2S2O4, acidified by AcOH, and refluxed 15 min. with 2 g. I, aged, filtered, and the precipitate refluxed 15 min. with 20 cc. N NaOH, diluted, and acidified, gives 0.6 g. 8-methyl-2,4,7-trioxohexahydropteridine-6-carboxylic acid. 1,3-Dimethyl-5-amino-4-methylaminouracil (2 g.) with 2.5 g. I in 25 cc. H2O refluxed 10 min., then cooled, gives 1.8 g. Et 1,3,8-trimethyl-2,4,7-trioxohexahydropteridine-6-carboxylate, m. 239°. This (1 g.) shaken 12 hrs. at 40° with 10 cc. N Na2CO3, then acidified with 5N H2SO4, gives 0.5 g. acid (hydrate), m. 160-2°, resolidifying then m. 200-10° (decomposition), anhydrous m. 215°. Methylation of 1,3-dimethyl -7-hydroxy-2,4-dioxotetrahydropteridine-6-carboxylic acid (II) (C.A. 49, 10324d) by CH2N2 in MeOHEt2O gives Me 1,3-dimethyl-7-methoxy-2,4-dioxotetrahydropteridine-6-carboxylate (III), m. 245-6°. III is also obtained from the Et ester of II and CH2N2. Hydrolysis of 0.5 g. III in 25 cc. N NaHCO3 during 2 days at 40°, then acidification of the warmed solution, gives 0.3 g. 1,3-dimethyl-7-methoxy -2,4-dioxotetrahydropteridine-6-carboxylic acid, m. 210° (decomposition).
IT Ionization
Ultraviolet and visible, spectra
(of 1,2,3,4-tetrahydro-7-hydroxy-2,4-dioxo-6-pteridinecarboxylic acid and derivs.)
IT 2,4,6(1H,3H,5H)-Pteridinetrione, 1,3,7-trimethyl-
7-Pteridinecarboxylic acid, 1,2,3,4,5,6-hexahydro-3-methyl-2,4-dioxo-
IT 33744-31-9, 6-Pteridinecarboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-2,4-dioxo- 89642-07-9, 7-Pteridinecarboxylic acid, 1,2,3,4,5,6-hexahydro-2,4,6-trioxo-
(and derivs.)
IT 90321-74-7, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-8-methyl-2,4,7-trioxo- **91769-67-4**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester **99073-13-9**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- 100949-11-9, 6-Pteridinecarboxylic acid,

1,2,3,4-tetrahydro-7-hydroxy-3-methyl-2,4-dioxo- 100949-42-6, 6-Pteridinecarboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-1-methyl-2,4-dioxo- 101872-28-0, 6-Pteridinecarboxylic acid, 1,2,3,4-tetrahydro-7-methoxy-1,3-dimethyl-2,4-dioxo- 104095-10-5, 6-Pteridinecarboxylic acid, 1,2,3,4-tetrahydro-7-methoxy-1,3-dimethyl-2,4-dioxo-, methyl ester
(preparation of)

IT **91769-67-4**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester **99073-13-9**, 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-
(preparation of)

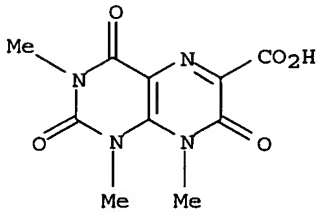
RN 91769-67-4 HCAPLUS

CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester (6CI, 7CI) (CA INDEX NAME)



RN 99073-13-9 HCAPLUS

CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (6CI) (CA INDEX NAME)



L59 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1958:104358 HCAPLUS

DN 52:104358

OREF 52:18458b-h

ED Entered STN: 22 Apr 2001

TI Pteridines. II. 7-Hydroxy-and 7-hydroxy-6-methyl-2,4-dioxotetrahydropteridines

AU Pfleiderer, Wolfgang

CS Tech. Hochschule, Stuttgart, Germany

SO Chemische Berichte (1957), 90, 2588-603
CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA Unavailable

CC 10G (Organic Chemistry: Heterocyclic Compounds)

AB The synthesis of 7-hydroxypteridines is greatly improved by isolation of the intermediate anils. The structure of the products is shown by spectra and by the acid strengths; 7-OH ionizes first, then N1- then N3-H. A suspension of 2.8 g. 4,5-diaminouracil (I) in 250 cc.H2O shaken with 4 g. EtO2CCH(OH)OEt (II) gives 3.5 g. Et 4-aminouracil-5-azomethinecarboxylate (III), which sinters at 235°. Similarly are prepared the 3-methyl (m. 225°) and 1-methyl (m. 231° decomposition) derivs., and Et 1,3 -dimethyl-4-methylaminouracil-5-azomethinecarboxylate (IV), m. 186°. III (3 g.) refluxed 30 min. with 75 cc. N NaHCO3, then diluted

with 75 cc. H2O, filtered hot, and added to 200 cc. boiling 0.5N HCl, gives 2.2 g. 7-hydroxy-2,4-dioxotetrahydropteridine. Similarly the 3-methyl and 1-methyl derivs. are prepared IV (1.2 g.) refluxed 2 hrs. in 36 cc. H2O, then evaporated in vacuo, gives 0.5 g. 1,3,8-trimethyl-2,4,7-trioxohexahydropteridine, m. 220°. 5-Nitroso-4-methylaminouracil (V) (1.2 g.) is reduced with Na2S2O4 in alkaline solution, acidified with AcOH, and treated with 1.5 g. II. The precipitate is filtered off, boiled 15 min. with 30 cc. N NaHCO3, the precipitated Na salt filtered off, dissolved in 50 cc. H2O, and added to boiling dilute HCl to precipitate 0.7 g. 8-methyl-2,4,7-trioxohexahydropteridine. A fine suspension of 1 g. 1,3-dimethyl-7-hydroxy-2,4-dioxotetrahydropteridine (C.A. 49, 10324d) in 100 cc. absolute MeOH and Et2O with CH2N2 gives 0.4 g. 1,3-dimethyl-7-methoxy-2,4-dioxotetrahydropteridine, m. 195-6°. The same product is obtained using Me2SO4 in N NaOH. 2,4,5-Triamino-6-hydroxypyrimidine (VI) (2.8 g.) in 500 cc. H2O shaken with 5 cc. II yields 4.1 g. Et 2,4-diamino-6-hydroxypyrimidine-5-azomethinecarboxylate. This is refluxed 10 min. with 82 cc. 0.5N NaHCO3, the precipitate filtered off, dissolved in dilute NaOH, and precipitated by HCl to give 2 g. isoxanthopterin. I (1.4 g.) in 50 cc. H2O refluxed 15 min. with 1 g. AcCO2Me gives 1.2 g. 7-hydroxy-6-methyl-2,4-dioxotetrahydropteridine; similarly the 1,6-dimethyl (decompose from 330°) and 3,6-dimethyl derivs. are prepared V (1.2 g.) reduced and treated with AcOH and AcCO2Me, refluxed 15 min., then aged 12 hrs., gives 0.7 g. 6,8-dimethyl-2,4,7-trioxohexahydropteridine. 1,3-Dimethyl-5-amino-4-methylaminouracil (1.8 g.) in 20 cc. H2O boiled 15 min. with 1.2 g. AcCO2Me gives 1,3,6,8-tetramethyl-2,4,7-trioxohexahydropteridine, m. 253°, sublimed in vacuo at 200°. Methylation of 1,3,6-trimethyl-7-hydroxy-2,4-dioxotetrahydropteridine (C.A. 51, 437c) by CH2N2 in MeOH-Et2O or by Me2SO4 gives 1,3,6-trimethyl-7-methoxy-2,4-dioxotetrahydropteridine, m. 241°. VI with AcCO2Me gives 6-methylisoxanthopterin.

IT Ionization
Ultraviolet and visible, spectra
(of 7-hydroxylumazine and derivs.)

IT 2577-35-7, 2,4,6(1H,3H,5H)-Pteridinetrione 2577-38-0, Lumazine, 7-hydroxy- 14868-37-2, 2,4,6(1H,3H,5H)-Pteridinetrione, 7-methyl- 31053-46-0, Lumazine, 7-hydroxy-6-methyl-
(and derivs.)

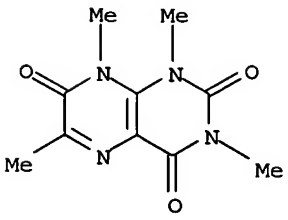
IT 529-69-1, Isoxanthopterin 712-38-9, 4,7-Pteridinediol, 2-amino-6-methyl- 2614-42-8, Lumazine, 7-methoxy-1,3-dimethyl- 2614-43-9, Lumazine, 7-hydroxy-1,3-dimethyl- 2614-44-0, Lumazine, 7-hydroxy-1-methyl- 2622-65-3, Lumazine, 7-hydroxy-3-methyl- 2622-66-4, Lumazine, 7-methoxy-1,3,6-trimethyl- 2625-22-1, Lumazine, 7-hydroxy-1,6-dimethyl- 2625-23-2, Lumazine, 7-hydroxy-3,6-dimethyl- 6743-25-5, 2,4,7(1H,3H,8H)-Pteridinetrione, 6,8-dimethyl- 19845-00-2, 2,4,7(1H,3H,8H)-Pteridinetrione, 8-methyl- 70674-01-0, Formic acid, [N-(1,2,3,4-tetrahydro-1,3-dimethyl-6-methylamino-2,4-dioxo-5-pyrimidinyl)formimidoyl]-, ethyl ester 70674-02-1, 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,8-trimethyl- **99069-70-2**, 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl- 102369-85-7, Formic acid, [N-(6-amino-1,2,3,4-tetrahydro-1-methyl-2,4-dioxo-5-pyrimidinyl)formimidoyl]-, ethyl ester 102369-85-7, Acetic acid, (6-amino-1,2,3,4-tetrahydro-1-methyl-2,4-dioxo-5-pyrimidinylimino)-, ethyl ester 106166-66-9, Formic acid, [N-(6-amino-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)formimidoyl]-, ethyl ester 106166-66-9, Acetic acid, (6-amino-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinylimino)-, ethyl ester 113476-31-6, Formic acid, [N-(4-amino-1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-5-pyrimidinyl)formimidoyl]-, ethyl ester 113476-31-6, Acetic acid, (4-amino-1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-5-pyrimidinylimino)-, ethyl ester 117123-36-1, Acetic acid, (2,4-diamino-6-hydroxy-5-pyrimidinylimino)-, ethyl ester 117123-36-1, Formic acid, [N-(2,4-diamino-6-hydroxy-5-pyrimidinyl)formimidoyl]-, ethyl ester
(preparation of)

IT **99069-70-2**, 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl-
(preparation of)

RN 99069-70-2 HCAPLUS

CN 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl- (6CI, 9CI) (CA

INDEX NAME)



L59 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1958:104357 HCAPLUS
DN 52:104357
OREF 52:**18457h-i,18458a-b**
ED Entered STN: 22 Apr 2001
TI Pteridines. I. 2,4-Dioxotetrahydropteridines
AU Pfleiderer, Wolfgang
CS Tech. Hochschule, Stuttgart, Germany
SO Chemische Berichte (1957), 90, 2582-7
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
AB In each of the following papers the ultraviolet spectra, pKa values, paper chromatographic characteristics, and fluorescence of a group of pteridines are tabulated. The structures assigned are based (with respect to lactam-lactim tautomerism) on comparison of the spectra of the parent compound with those of the O-and N-Me derivs. The order of ionization of the H atoms is determined by comparing spectra of partly ionized compds. with those of the Me derivs. M.ps. "above 350°" are reported except where indicated in the abstract 3-Methyl-4,5-diaminouracil hydrochloride (1 g.) refluxed 1 hr. with 1.5 g. glyoxal sodium bisulfite in 20 cc. 0.5N HCl, filtered, evaporated in vacuo and the residue sublimed in vacuo, gives 0.4 g. 1-methyllumazine, m. 290-1°. 3-Methyllumazine is prepared similarly, m. 332°. A solution of 1.7 g. 1-methyl-2-methoxy-4,5-diamino-6-oxodihydropyrimidine in 50 cc. absolute MeOH is treated with gaseous (CHO)2 (from 3 g. polymer and 15 g. P2O5), refluxed 10 min., filtered hot, and the residue crystallized from a large volume of Et2O to give 0.7 g. glyoxal bis(1-methyl-2-methoxy-4,5-diamino-6-oxodihydropyrimidine), yellow, m. 235°. The MeOH filtrate is evaporated to give 0.5 g. 3-methyl-2-methoxy-4-oxodihydropteridine, m.p. 190°. 5-Nitro-2,6-dimethoxy-4-aminopteridine (3 g.) in 270 cc. absolute MeOH hydrogenated with Raney Ni, the solution concentrated to 50 cc., and the residue treated with (CHO)2 (4 g. polyglyoxal) at room temperature, and filtered, gives 1.8 g. glyoxal bis(2,6-dimethoxy-4,5-diaminopyrimidine), m. 229° (decomposition). Evaporation of the filtrate gives 0.6 g. 2,4-dimethoxypteridine, m. 200°. A suspension of 1 g. powdered lumazine in 75 cc. absolute MeOH with Et2O-CH2N2 [from 10 g. MeN(NO)CONH2] dissolves and then (12 hrs.) ppts. as 0.15 g. 1,3-dimethyl-2,4-dioxotetrahydropteridine, m. 200°. The structure 2,4-dioxotetrahydropteridine is assigned to lumazine; N1-H ionizes first, then N3-H.
IT Fluorescence
Ultraviolet and visible, spectra
(of pteridine derivs.)
IT Ionization
(of pteridines)
IT 4(3H)-Pyrimidinone, (ethanediylidenedinitrilo)bis[amino-2-methoxy-3-methyl-
IT 487-21-8, Lumazine 2577-38-0, Lumazine, 7-hydroxy- 31053-46-0, Lumazine, 7-hydroxy-6-methyl-
(and derivs.)
IT 91-18-9, Pteridine
(derivs.)

IT 13401-18-8, Lumazine, 1,3-dimethyl- 50256-18-3, Lumazine, 1-methyl-
50256-19-4, Lumazine, 3-methyl- 99584-93-7, 4(3H)-Pteridinone,
2-methoxy-3-methyl- 108128-86-5, Pteridine, 2,4-dimethoxy-
109338-18-3, Pyrimidine, 5,5'-(ethanediylidenedinitrilo)bis[4-amino-2,6-
dimethoxy-
(preparation of)

=> b hcao
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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate
substance identification. Title keywords, authors, patent
assignees, and patent information, e.g., patent numbers, are
now searchable from 1907-1966. TIFF images of CA abstracts
printed between 1907-1966 are available in the PAGE
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all substance data from the REGISTRY file. Enter HELP FIRST for
more information.

=> d all l54 tot

L54 ANSWER 1 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA65:2260c CAOLD
TI pteridine studies - (XXXI) covalent hydration and subsequent oxidation of
8-methyl derivs. of some amino- and hydroxypteridines
AU Jacobsen, N. W.
IT 91-18-9 1603-79-8 4388-87-8 6743-13-1 6743-14-2 6743-15-3
6743-16-4 6743-17-5 6743-18-6 6743-19-7 6743-21-1 6743-22-2
6743-24-4 6743-25-5 6743-26-6 6743-27-7 6743-28-8
6743-29-9 6743-30-2 6743-31-3 6743-33-5 6743-34-6 6743-35-7
6743-36-8 6828-59-7 13530-12-6 31937-02-7

L54 ANSWER 2 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA61:7024h CAOLD
TI pyrido[2,3-d]pyrimidine-2,4,5,7-tetraones
AU Scarborough, Homer C.
PA Mead Johnson & Co.
DT Patent

PATENT NO.	KIND	DATE
US 3139432		1964
GB 989048		

IT 91996-75-7 93117-36-3 93738-66-0 93738-67-1 95709-04-9 96986-13-9
97360-49-1

L54 ANSWER 3 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA60:8027f CAOLD
TI pyrano[2,3-d]-and pyrido[2,3-d]pyrimidines
AU Scarborough, Homer C.
IT 90417-86-0 90559-74-3 90916-08-8 92058-18-9 92848-56-1 93117-36-3
93738-66-0 93738-67-1 95709-05-0 96986-13-9
97360-49-1

L54 ANSWER 4 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN

AN CA57:8569g CAOLD
TI pteridines - (XXI) synthesis and structure of 8-substituted 2,4,7-trioxohexahydropteridine-6-carboxylic acids
AU Nuebel, Gotthard; Pfleiderer, W.
IT 4318-56-3 5759-63-7 5759-79-5 5770-19-4 5770-20-7 17801-82-0
19845-00-2 21236-97-5 70404-26-1 89977-69-5 90321-74-7 90324-11-1
90324-12-2 90324-20-2 90917-19-4 91141-83-2 91687-86-4
91769-67-4 91823-54-0 92061-33-1 **93318-04-8**
95296-09-6 95766-75-9

L54 ANSWER 5 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA53:1364f CAOLD
TI pteridines - (VII) methylations of hydroxypteridines
AU Pfleiderer, Wolfgang
IT 2577-38-0 2614-42-8 2614-43-9 2614-44-0 2622-65-3 2625-21-0
3007-31-6 4088-36-2 6743-25-5 **6743-26-6** 19845-00-2
31053-46-0 63019-15-8 70916-39-1 70916-40-4 86488-48-4 99587-06-1
100974-92-3 102589-22-0 108128-89-8 108989-62-4 109187-19-1 110251-58-6

L54 ANSWER 6 OF 6 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA52:18457h CAOLD
TI pteridines - (I) 2,4-dioxotetrahydropteridines, (II) 7-hydroxy- and 7-hydroxy-6-methyl-2,-4-dioxotetrahydropteridines, (III) 2,4,6-trioxohexahydropteridines and the homologous 7-methyl derivs., (IV) 7-hydroxy-2,4-dioxotetrahydropteridine-6-carboxylic acids, (V) 2,4,6-trioxohexahydropteridine-7-carboxylic acids, (VI) 2,4,6,7-tetraoxooctahydropteridines
AU Pfleiderer, Wolfgang
IT 487-21-8 529-69-1 712-38-9 2577-35-7 2577-38-0 2614-42-8
2614-43-9 2622-66-4 2625-22-1 2625-23-2 2757-91-7 5770-48-9
6743-25-5 13401-18-8 14868-37-2 19845-00-2 31053-46-0 33744-31-9
50256-18-3 50256-19-4 50996-37-7 58947-87-8 61846-18-2 64724-39-6
70674-01-0 70674-02-1 89642-07-9 90004-69-6 90321-74-7 90350-04-2
90350-05-3 **91769-67-4** 92474-93-6 98277-38-4 99056-87-8
99069-70-2 **99073-13-9** 99584-42-6 99584-43-7
99584-93-7 100949-11-9 100949-42-6 101130-63-6 101580-61-4 101872-28-0
102369-85-7 103027-38-9 103030-02-0 103262-72-2 104095-10-5 106166-66-9
107057-43-2 108106-11-2 108106-88-3 108128-86-5 108850-68-6 109338-18-3
109868-91-9 113222-42-7 113222-44-9 113476-31-6 114062-77-0 114062-78-1
114062-82-7 115919-30-7 119276-65-2

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STRUCTURE FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9
DICTIONARY FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9

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****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *

* available and contains the CA role and document type information. *
*   *
****

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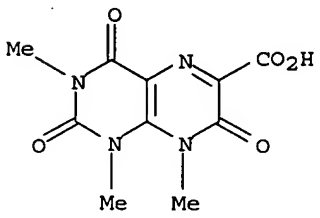
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l60 tot

L60 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **99073-13-9** REGISTRY
ED Entered STN: 16 Nov 1985
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H10 N4 O5
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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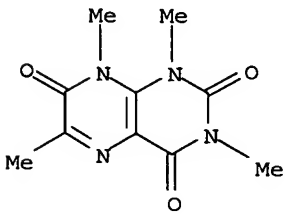
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **99069-70-2** REGISTRY
ED Entered STN: 16 Nov 1985
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 1,3,6,8-tetramethyl- (6CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H12 N4 O3
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT
(*File contains numerically searchable property data)



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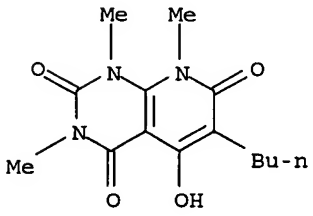
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **97360-49-1** REGISTRY
ED Entered STN: 27 Jul 1985
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 6-butyl-5-hydroxy-1,3,8-trimethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H19 N3 O4
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)



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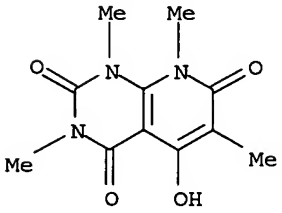
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **95709-05-0** REGISTRY
ED Entered STN: 06 Apr 1985
CN Pyrido[2,3-d]pyrimidine-2,4,7(1H,3H,8H)-trione, 5-hydroxy-1,3,6,8-tetramethyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H13 N3 O4
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT
(*File contains numerically searchable property data)



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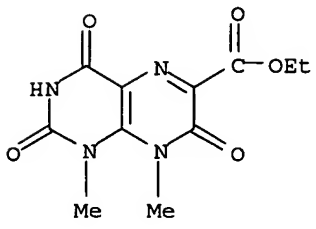
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **95296-09-6** REGISTRY
ED Entered STN: 16 Mar 1985
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-

trioxo-, ethyl ester (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H12 N4 O5
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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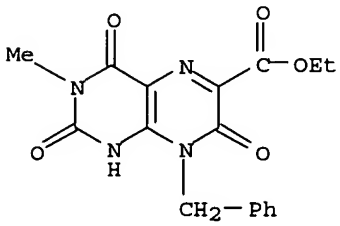
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **93318-04-8** REGISTRY
ED Entered STN: 18 Dec 1984
CN 6-Pteridinecarboxylic acid, 8-benzyl-1,2,3,4,7,8-hexahydro-3-methyl-2,4,7-trioxo-, ethyl ester (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N4 O5
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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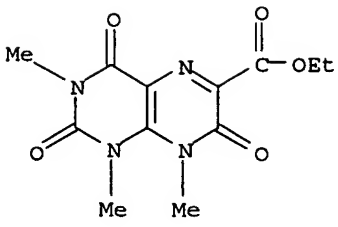
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **91769-67-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,3,8-trimethyl-2,4,7-trioxo-, ethyl ester (6CI, 7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 N4 O5
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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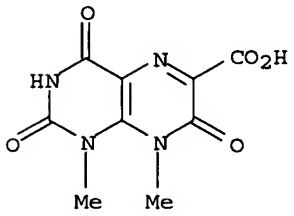
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

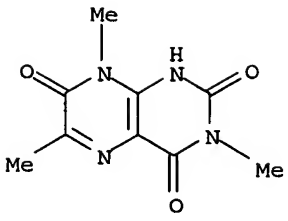
L60 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **90324-12-2** REGISTRY
ED Entered STN: 16 Nov 1984
CN 6-Pteridinecarboxylic acid, 1,2,3,4,7,8-hexahydro-1,8-dimethyl-2,4,7-trioxo- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H8 N4 O5
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L60 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **6743-26-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,4,7(1H,3H,8H)-Pteridinetrione, 3,6,8-trimethyl- (6CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7(3H,8H)-Pteridinedione, 2-hydroxy-3,6,8-trimethyl- (7CI, 8CI)
FS 3D CONCORD
MF C9 H10 N4 O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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